Coulomb Wave Functions in the Transition Region*

MILTON ABRAMOWITZ, *Computation Laboratory, National Bureau of Standards, Washington, D. C.*

AND

H. A. ANTOSIEWICZ, *Mathematics Department, The American University, Washington, D. C.*

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Expansions, involving the Airy integrals, of the functions $F_L(\eta,\rho)$, $G_L(\eta,\rho)$ are obtained from a study of the Coulomb wave equation. These expansions are convergent in the region $|\rho-\rho_1|<\rho_1$, where

$$\rho_1=\eta+[\eta^2+L(L+1)]^{\frac{1}{2}}.$$

1. INTRODUCTION

THE Coulomb wave functions $F_L(\eta,\rho)$, $G_L(\eta,\rho)$ which are defined as two linearly independent solutions of the differential equation

$$\frac{d^2y}{d\rho^2}+\left(1-\frac{2\eta}{\rho}-\frac{L(L+1)}{\rho^2}\right)y=0, \tag{1}$$

where L is a non-negative integer and $\eta>0$ is a parameter,[1] are of importance in many problems such as the separation of Schrödinger's wave equation for a Coulomb force field, the scattering of charged particles and the stability of laminar Poiseuille flow. They have been investigated intensively for the past several years and expansions of them have been obtained by various authors.[2]

In the present note, we establish first a representation of the general solution of (1) with $L=0$, valid in the region $|\rho-2\eta|<2\eta$, in terms of the well-known Airy integrals $\mathrm{Ai}(z)$, $\mathrm{Bi}(z)$ which, for $z\geq 0$, are defined[3] by the relations

$$\begin{aligned}\mathrm{Ai}(z)&=\tfrac{1}{3}z^{\frac{1}{2}}\{I_{-\frac{1}{3}}(\tfrac{2}{3}z^{\frac{3}{2}})-I_{\frac{1}{3}}(\tfrac{2}{3}z^{\frac{3}{2}})\},\\ \mathrm{Bi}(z)&=(z/3)^{\frac{1}{2}}\{I_{-\frac{1}{3}}(\tfrac{2}{3}z^{\frac{3}{2}})+I_{\frac{1}{3}}(\tfrac{2}{3}z^{\frac{3}{2}})\},\end{aligned} \tag{2}$$

where $I_{\pm\frac{1}{3}}(x)$ is the modified Bessel function of the first kind. We then outline our method briefly for the case $L\neq 0$ and not necessarily an integer. As far as the functions $F_L(\eta,\rho)$, $G_L(\eta,\rho)$ are concerned, there is no real loss of generality in considering the case $L=0$ only as these functions satisfy recurrence relations by which they can be generated from the functions $F_0(\eta,\rho)$, $G_0(\eta,\rho)$ and their derivatives.

The possibility of a representation of the solutions of (1) with $L=0$ in terms of Airy integrals becomes apparent if we transform Eq. (1) by the substitution

$$x=(2\eta-\rho)/(2\eta)^{\frac{1}{3}},\quad \mu=(2\eta)^{\frac{2}{3}}, \tag{3}$$

into the equation

$$y''-\frac{\mu x}{\mu-x}y=0; \tag{4}$$

for this equation resembles, the more so the larger μ, the equation

$$u''-xu=0, \tag{5}$$

whose general solution may be written in the form

$$u(x)=c_1\,\mathrm{Ai}(x)+c_2\,\mathrm{Bi}(x). \tag{6}$$

It seems reasonable, therefore, to presume that the general solution of (4) may be represented for all $\mu\neq 0$ in the form $y(x,\mu)=Y(x,\mu)u(x)$, where $Y(x,\mu)$ is suitably determined. Indeed, such a representation is possible but rather awkward to obtain. Rather, we attempt to find a representation in the form

$$y(x,\mu)=\phi(x,\mu)u(x)+\psi(x,\mu)u'(x), \tag{7}$$

where $u(x)$ is defined as in (6). This, as we shall see, will enable us to determine the functions $\phi(x,\mu)$, $\psi(x,\mu)$ as analytic functions of x for all $|x|\leq r<|\mu|$ whose series expansions have coefficients that are readily available from simple algebraic recurrence relations. It is this fact which makes the representation (7) extremely useful for numerical computations since the error in truncating the series expansions of $\phi(x,\mu)$, $\psi(x,\mu)$ can be estimated from a comparison with the expansion of $1/(1-x/\mu)$.

2. REPRESENTATION OF $y(x,\mu)$

Let

$$\begin{aligned}y_1(x,\mu)&=\phi(x,\mu)\,\mathrm{Ai}(x)+\psi(x,\mu)\,\mathrm{Ai}'(x),\\ y_2(x,\mu)&=\phi(x,\mu)\,\mathrm{Bi}(x)+\psi(x,\mu)\,\mathrm{Bi}'(x).\end{aligned} \tag{8}$$

We wish to determine the functions $\phi(x,\mu)$, $\psi(x,\mu)$ such that for every $\mu\neq 0$ and x in $|x|\leq r<|\mu|$ the functions $y_1(x,\mu)$, $y_2(x,\mu)$ are two linearly independent solutions of (4).

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[1] *Tables of Coulomb Wave Functions*, National Bureau of Standards, Applied Mathematics Series 17 (U. S. Government Printing Office, Washington, D. C., 1952), Vol. 1.

[2] See, e.g., Bloch, Hull, Broyles, Bouricius, Freeman, and Breit, Phys. Rev. **80**, 553 (1950); T. D. Newton, Atomic Energy of Canada, Limited. Unclassified Report, CRT-526 (unpublished).

[3] *The Airy Integral* (British Association for the Advancement of Science, Cambridge, 1946).

On substituting either of the expressions (8) into Eq. (4) and equating to zero the coefficients of the respective Airy integral and its derivative, we obtain the system of differential equations,

$$\phi''-\frac{x^2}{\mu-x}\phi+2x\psi'+\psi=0,\quad \psi''-\frac{x^2}{\mu-x}\psi+2\phi'=0,\quad (9)$$

which we attempt to solve for $|x|\leq r<|\mu|$ by assuming that $\phi(x,\mu)$, $\psi(x,\mu)$ admit the expansions

$$\phi(x,\mu)=\sum_0^\infty a_n(\mu)x^n,\quad \psi(x,\mu)=\sum_0^\infty b_n(\mu)x^n.\quad (10)$$

Expanding $x^2/(\mu-x)$ in (9) in powers of x, we thus find the recurrence relations

$$\begin{aligned} a_2&=-\tfrac{1}{2}b_0, & a_3&=-\tfrac{1}{2}b_1,\\ b_2&=-a_1, & b_3&=\tfrac{2}{3}a_2, \end{aligned}\quad (11)$$

$$\begin{aligned} a_{n+4}&=\frac{1}{(n+4)(n+3)}\left\{\sum_0^n \mu^{-j-1}a_{n-j}-(2n+5)b_{n+2}\right\},\\ b_{n+4}&=\frac{1}{(n+4)(n+3)}\left\{\sum_0^n \mu^{-j-1}b_{n-j}-2(n+3)a_{n+3}\right\},\\ &n=0,\,1,\,2,\,\cdots. \end{aligned}\quad (12)$$

Hence, the four constants a_0, a_1, b_0, b_1 are arbitrary within the restriction that $y_1(x,\mu)$, $y_2(x,\mu)$ be linearly independent. The simplest choice, satisfying this requirement, is to take

$$a_0=1,\quad a_1=b_0=b_1=0,\quad (13)$$

whence it follows that the Wronskian determinant of $y_1(x,\mu)$, $y_2(x,\mu)$ at $x=0$ becomes $W[y_1,y_2]=\pi^{-1}$. For convenience, we list a few terms in the resulting expansions (10):

$$\begin{aligned} \phi(x,\mu)&=1+\frac{1}{12\mu}x^4+\frac{1}{20\mu^2}x^5+\frac{1}{30\mu^3}x^6\\ &\quad+\frac{1}{42}\left(\frac{1}{\mu^4}+\frac{11}{30\mu}\right)x^7+\cdots,\\ \psi(x,\mu)&=-\frac{1}{30\mu}x^5-\frac{1}{60\mu^2}x^6-\frac{1}{105\mu^3}x^7\\ &\quad-\frac{1}{168}\left(\frac{1}{\mu^4}+\frac{11}{30\mu}\right)x^8+\cdots. \end{aligned}\quad (14)$$

Since the coefficients in the system (9) are analytic functions of x for all $|x|\leq r<|\mu|$, it follows from a well-known theorem that its solutions are likewise analytic functions of x for all $|x|\leq r<|\mu|$. Thus, the functions $\phi(x,\mu)$, $\psi(x,\mu)$ as defined in (14) are for every $\mu\neq 0$ analytic in x for all $|x|\leq r<|\mu|$.

3. CONCLUSION

The determination of a particular solution of Eq. (4) is straightforward. Choosing, for instance, $x=0$ as initial point, we obtain for the constants involved in the representation (7):

$$\begin{aligned} c_1&=\pi\sqrt{3}\{y'(0,\mu)\ \mathrm{Ai}(0)-y(0,\mu)\ \mathrm{Ai}'(0)\},\\ c_2&=-\pi\{y'(0,\mu)\ \mathrm{Ai}(0)+y(0,\mu)\ \mathrm{Ai}'(0)\}. \end{aligned}\quad (15)$$

If we put $y(0,\mu)=F_0(\eta,2\eta)$, $y'(0,\mu)=(2\eta)^{\frac{1}{3}}(dF_0/d\rho)_{\rho=2\eta}$, these constants normalize (7) to represent $F_0(\eta,\rho)$ for all ρ in the region $|\rho-2\eta|<2\eta$, $\eta>0$; a similar set of constants may be obtained for $G_0(\eta,\rho)$.[4]

If $L\neq 0$ we can derive an analogous representation. Indeed, if in (1), we let

$$x=(\rho_1-\rho)/\rho_1^{\frac{1}{3}},\quad \nu=\rho_1^{\frac{2}{3}},\quad (16)$$

where ρ_1 is the larger of the two roots (assumed to be real) of the equation

$$\rho^2-2\eta\rho-L(L+1)=0,\quad (17)$$

namely,

$$\rho_{1,\,2}=\eta\pm[\eta^2+L(L+1)]^{\frac{1}{2}},\quad (18)$$

we obtain the equation

$$\frac{d^2y}{dx^2}-\left\{\frac{\nu x}{\nu-x}-\frac{L(L+1)x}{\nu(\nu-x)^2}\right\}y=0,\quad (19)$$

whose "limiting" equation as $\nu\to\infty$ is

$$(d^2u/dx^2)-xu=0.\quad (20)$$

The above method yields the representation

$$y(x,\nu,L)=\phi_L(x,\nu)u(x)+\psi_L(x,\nu)u'(x),\quad (21)$$

where $u(x)$ is defined as in (6) and

$$\begin{aligned} \phi_L(x,\nu)&=\sum_0^\infty \alpha_n(\nu,L)x^n=1-\frac{L(L+1)}{6\nu^4}x^3+\cdots,\\ \psi_L(x,\nu)&=\sum_0^\infty \beta_n(\nu,L)x^n=\frac{L(L+1)}{12\nu^4}x^4+\cdots, \end{aligned}\quad (22)$$

with coefficients determined as follows:

$$\begin{aligned} &\alpha_0=1,\quad \alpha_1=\alpha_2=0,\quad \alpha_3=-L(L+1)/6\nu^4,\\ &\beta_0=\beta_1=\beta_2=\beta_3=0,\\ &\alpha_{n+4}=\frac{1}{(n+4)(n+3)}\left\{\sum_0^n \nu^{-j-1}\alpha_{n-j}-(2n+5)\beta_{n+2}\right.\\ &\qquad\left.-L(L+1)\sum_0^{n+2} j\nu^{-j-3}\alpha_{n+2-j}\right\},\quad (23) \end{aligned}$$

[4] Asymptotic expansions of $F_0(\eta,2\eta)$, $G_0(\eta,2\eta)$ were obtained in the following paper: [M. Abramowitz and P. Rabinowitz, Phys. Rev. **96**, 77 (1954)].

$$\beta_{n+4}=\frac{1}{(n+4)(n+3)}\left\{\sum_0^n \nu^{-j-1}\beta_{n-j}-(2n+6)\alpha_{n+3}\right.$$
$$\left.-L(L+1)\sum_0^{n+2} j\nu^{-j-3}\beta_{n+2-j}\right\},$$
$$n=0,1,2,\cdots.$$

The functions $\phi_L(x,\nu)$, $\psi_L(x,\nu)$ are analytic in x for all $|x|<\nu$, i.e., $|\rho-\rho_1|<\rho_1$. Note that by (18) $\rho_1\to\infty$ with η while $\rho_2\to 0$ as $\eta\to\infty$, L being fixed.

The above results are contained in a general representation theorem for the solutions of an nth order linear ordinary differential equation with analytic coefficients.[5]

[5] H. A. Antosiewicz and M. Abramowitz, "A Representation for Solutions of Analytic Systems of Linear Differential Equations," J. Wash. Acad. Sci. (to be published).

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Evaluation of Coulomb Wave Functions along the Transition Line*

MILTON ABRAMOWITZ AND PHILIP RABINOWITZ
Computation Laboratory, National Bureau of Standards, Washington, D. C.
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Asymptotic representations are obtained for the regular and irregular Coulomb wave functions and their derivatives for $\rho=2\eta$. A table of these functions is given, and a discussion is given to show how values may be obtained for $\rho\neq 2\eta$ by using Taylor's formula.

In a recent paper Barfield and Broyles[1] evaluated the Coulomb wave functions F_0, G_0, and F_0' from their contour integral representations for $\rho=2\eta$ and gave a short table of these functions. They made the observation that a knowledge of the functions for $\rho=2\eta$ permitted the efficient use of local Taylor expansions for numerical computation. It is the purpose of this paper to exploit these suggestions and demonstrate a systematic method of computation over a wide range of values of ρ and η. Specifically, we provide in Table I values of these functions for 2η ranging from 0 to 50 and develop an asymptotic formula which may be used for larger values of the argument. The tabular values were computed on the National Bureau of Standards SEAC with the aid of programs prepared by Dr. C. E. Froberg of Sweden during his stay at the Computation Laboratory of the National Bureau of Standards. The results were obtained to nine decimal places by numerical quadrature of integral representations of the functions and checks were applied by differencing and calculation of the Wronskian. The table as given to seven decimals is correct to within a unit of the last place. The intervals were chosen so that the five-point Lagrangian interpolation formula will yield the full accuracy beyond $\rho=3$. For larger values of 2η, the representations obtained will yield equivalent results.

We restrict our discussion to the case $L=0$ since there is a convenient method of generating the functional values for $L>0$ for the pertinent range of values of ρ and η with the aid of the recurrence relations.

We start with the integral representation[2] employed by Newton,

$$F_0-iG_0=\rho C_0(\eta)\int_{-1}^{-i\infty}\exp(2\eta i\,\mathrm{arctanh}s-i\rho s)ds,\quad (1)$$

where $C_0(\eta)=(2\pi\eta)^{-\frac{1}{2}}(1-e^{-2\pi\eta})^{-\frac{1}{2}}$, in order to obtain asymptotic expansions for F_0 and G_0 and their derivatives for $\rho=2\eta$. In this case, we have

$$F_0(2\eta)-iG_0(2\eta)=2\eta C_0\int_{-1}^{-i\infty}\exp[2\eta i(\mathrm{arctanh}s-s)]ds,\quad (2)$$

and evaluate this integral by the method of steepest descents. We note that if $f(s)=\mathrm{arctanh}s-s$, then $f'(s)$ has a double zero for $s=0$ and $f(s)=\frac{1}{3}s^3+\frac{1}{5}s^5+\cdots$. Thus, if $s=e^{i\theta}$, is^3 is real and negative for $\theta=5\pi/6$ and $\theta=-\pi/2$, the paths of steepest descent. We consequently deform the path from $s=-1$ to $s=-i\infty$ into the equivalent path

$$c_1:\quad s=e^{i\theta},\quad \pi\geq\theta\geq 5\pi/6;$$
$$c_2:\quad s=\zeta e^{5\pi i/6},\quad 1\geq\zeta\geq 0;\quad (3)$$
$$c_3:\quad s=\zeta e^{-\pi i/2},\quad 0\leq\zeta\leq\infty.$$

It can then be shown that the contribution from the integral along c_1 is smaller in absolute value than $\frac{1}{6}\pi\exp\{-\eta(\frac{1}{2}\pi\eta-1)\}$. The integral along c_3 is

$$J_3=-i\int_0^\infty\exp[2\eta(\arctan\zeta-\zeta)]d\zeta,\quad (4)$$

and this can be represented asymptotically by the

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[1] W. D. Barfield and A. A. Broyles, Phys. Rev. 88, 892 (1952).
[2] T. D. Newton, Chalk River Laboratory Report 526, December, 1952 (unpublished).