

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

$$n=0, 1, 2, \dots$$

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)  $\rho_1 \rightarrow \infty$  with  $\eta$  while  $\rho_2 \rightarrow 0$  as  $\eta \rightarrow \infty$ ,  $L$  being fixed.

The above results are contained in a general representation theorem for the solutions of an  $n$ th order linear ordinary differential equation with analytic coefficients.<sup>5</sup>

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

### Evaluation of Coulomb Wave Functions along the Transition Line\*

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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<sup>1</sup> 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  $\rho$  and  $\eta$ . Specifically, we provide in Table I values of these functions for  $2\eta$  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  $2\eta$ , 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  $\rho$  and  $\eta$  with the aid of the recurrence relations.

We start with the integral representation<sup>2</sup> employed

by Newton,

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

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

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

and evaluate this integral by the method of steepest descents. We note that if  $f(s) = \operatorname{arctanh} s - s$ , then  $f'(s)$  has a double zero for  $s = 0$  and  $f(s) = \frac{1}{3}s^3 + \frac{1}{5}s^5 + \dots$ . 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

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

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

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

and this can be represented asymptotically by the

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<sup>1</sup> W. D. Barfield and A. A. Broyles, Phys. Rev. **88**, 892 (1952).

<sup>2</sup> T. D. Newton, Chalk River Laboratory Report 526, December, 1952 (unpublished).

TABLE I. Coulomb functions for  $\rho=2\eta$ .

| $\rho=2\eta$ | $F_0$     | $F_0'$    | $G_0$     | $G_0'$     | $\rho=2\eta$ | $F_0$     | $F_0'$    | $G_0$     | $G_0'$     |
|--------------|-----------|-----------|-----------|------------|--------------|-----------|-----------|-----------|------------|
| 0.0          | 0.0000000 | 1.0000000 | 1.0000000 | 0.0000000  | 15.0         | 0.9847202 | 0.3052996 | 1.7171606 | -0.4831337 |
| 0.5          | 0.3485125 | 0.7251403 | 1.1482085 | -0.4802921 | 15.5         | 0.9902704 | 0.3033518 | 1.7263386 | -0.4809919 |
| 1.0          | 0.5166015 | 0.5929246 | 1.1974870 | -0.5613235 | 16.0         | 0.9956675 | 0.3014834 | 1.7352810 | -0.4789166 |
| 1.5          | 0.6065420 | 0.5232290 | 1.2379327 | -0.5807968 | 16.5         | 1.0009207 | 0.2996885 | 1.7440008 | -0.4769040 |
| 2.0          | 0.6617816 | 0.4815575 | 1.2757788 | -0.5827288 | 17.0         | 1.0060382 | 0.2979621 | 1.7525097 | -0.4749507 |
| 2.5          | 0.7004111 | 0.4535470 | 1.3106041 | -0.5790591 | 17.5         | 1.0110275 | 0.2962996 | 1.7608186 | -0.4730536 |
| 3.0          | 0.7301291 | 0.4330004 | 1.3422906 | -0.5735802 | 18.0         | 1.0158956 | 0.2946968 | 1.7689374 | -0.4712097 |
| 3.5          | 0.7544607 | 0.4169974 | 1.3711212 | -0.5676187 | 18.5         | 1.0206486 | 0.2931499 | 1.7768754 | -0.4694163 |
| 4.0          | 0.7751972 | 0.4040078 | 1.3974834 | -0.5616710 | 19.0         | 1.0252926 | 0.2916555 | 1.7846412 | -0.4676709 |
| 4.5          | 0.7933518 | 0.3931476 | 1.4217412 | -0.5559273 | 19.5         | 1.0298329 | 0.2902104 | 1.7922428 | -0.4659712 |
| 5.0          | 0.8095520 | 0.3838640 | 1.4442027 | -0.5504558 | 20           | 1.0342745 | 0.2888118 | 1.7996876 | -0.4643149 |
| 5.5          | 0.8242151 | 0.3757900 | 1.4651204 | -0.5452732 | 22           | 1.0511411 | 0.2836314 | 1.8280303 | -0.4580862 |
| 6.0          | 0.8376341 | 0.3686700 | 1.4847003 | -0.5403739 | 24           | 1.0667458 | 0.2790155 | 1.8543437 | -0.4524127 |
| 6.5          | 0.8500228 | 0.3623195 | 1.5031110 | -0.5357429 | 26           | 1.0812800 | 0.2748610 | 1.8789213 | -0.4472086 |
| 7.0          | 0.8615430 | 0.3566012 | 1.5204917 | -0.5313615 | 28           | 1.0948936 | 0.2710901 | 1.9019960 | -0.4424062 |
| 7.5          | 0.8723199 | 0.3514106 | 1.5369583 | -0.5272109 | 30           | 1.1077061 | 0.2676425 | 1.9237558 | -0.4379512 |
| 8.0          | 0.8824527 | 0.3466662 | 1.5526082 | -0.5232725 | 32           | 1.1198147 | 0.2644708 | 1.9443548 | -0.4337994 |
| 8.5          | 0.8920214 | 0.3423035 | 1.5675239 | -0.5195291 | 34           | 1.1312995 | 0.2615371 | 1.9639206 | -0.4299144 |
| 9.0          | 0.9010915 | 0.3382706 | 1.5817760 | -0.5159650 | 36           | 1.1422273 | 0.2588106 | 1.9825608 | -0.4262657 |
| 9.5          | 0.9097174 | 0.3345251 | 1.5954254 | -0.5125659 | 38           | 1.1526543 | 0.2562659 | 2.0003662 | -0.4228279 |
| 10.0         | 0.9179449 | 0.3310321 | 1.6085246 | -0.5093189 | 40           | 1.1626285 | 0.2538820 | 2.0174148 | -0.4195792 |
| 10.5         | 0.9258127 | 0.3277625 | 1.6211196 | -0.5062124 | 42           | 1.1721911 | 0.2516411 | 2.0337740 | -0.4165011 |
| 11.0         | 0.9333539 | 0.3246917 | 1.6332507 | -0.5032358 | 44           | 1.1813778 | 0.2495282 | 2.0495020 | -0.4135776 |
| 11.5         | 0.9405973 | 0.3217989 | 1.6449537 | -0.5003796 | 46           | 1.1902198 | 0.2475306 | 2.0646501 | -0.4107947 |
| 12.0         | 0.9475677 | 0.3190663 | 1.6562601 | -0.4976353 | 48           | 1.1987442 | 0.2456371 | 2.0792632 | -0.4081403 |
| 12.5         | 0.9542871 | 0.3164785 | 1.6671980 | -0.4949953 | 50           | 1.2069751 | 0.2438382 | 2.0933811 | -0.4056037 |
| 13.0         | 0.9607746 | 0.3140223 | 1.6777927 | -0.4924524 |              |           |           |           |            |
| 13.5         | 0.9670473 | 0.3116858 | 1.6880668 | -0.4900003 |              |           |           |           |            |
| 14.0         | 0.9731203 | 0.3094591 | 1.6980407 | -0.4876333 |              |           |           |           |            |
| 14.5         | 0.9790072 | 0.3073330 | 1.7077331 | -0.4853460 |              |           |           |           |            |

expansion

$$J_3 = \frac{-i}{3\beta} \left\{ \Gamma\left(\frac{1}{3}\right) + \sum_{n=5}^{\infty} \frac{a_n \Gamma\left(\frac{1}{3}n + \frac{1}{3}\right)}{\beta^n} \right\}, \quad \beta^3 = \frac{2}{3}\eta, \quad (5)$$

where the coefficients  $a_n$  are given recursively by

$$\begin{aligned} a_5 &= (3/5)\beta^3, \quad a_6 = 0, \quad a_7 = -(3/7)\beta^3, \\ a_8 &= 0, \quad a_9 = (1/3)\beta^3, \quad (6) \\ (n+2)a_{n+2} + na_n &= 3\beta^3 a_{n-3}. \end{aligned}$$

The integral along  $c_2$  can be evaluated in exactly the same manner.

If we collect our results, making use of the fact that

$$2\eta C_0 \cong (2\eta/\pi)^{\frac{1}{2}} = (3/\pi)^{\frac{1}{2}} \beta^{\frac{1}{2}},$$

we get

$$\begin{aligned} F_0(2\eta) &\cong \frac{\Gamma(\frac{1}{3})\beta^{\frac{1}{2}}}{2\sqrt{\pi}} \left\{ 1 - \frac{2}{35} \frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{1}{3})} \frac{1}{\beta^4} - \frac{8}{2025} \frac{1}{\beta^6} - \dots \right\}, \\ G_0(2\eta) &\cong \frac{\sqrt{3}\Gamma(\frac{1}{3})\beta^{\frac{1}{2}}}{2\sqrt{\pi}} \left\{ 1 + \frac{2}{35} \frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{1}{3})} \frac{1}{\beta^4} - \frac{8}{2025} \frac{1}{\beta^6} + \dots \right\}. \end{aligned} \quad (7)$$

The coefficient of  $\beta^{-8}$  in these expansions is zero, so that the error is smaller than  $\beta^{-10}$ .

The procedure may be carried out in an entirely similar manner to determine  $F_0'$  and  $G_0'$ , since from (1) we get

$$\begin{aligned} \frac{dF_0}{d\rho} - i \frac{dG_0}{d\rho} &= -\frac{1}{\rho} (F_0 - iG_0) \\ &= -i\rho C_0 \int_{-1}^{-i\infty} \exp(2\eta i \operatorname{arctanh}s - i\rho s) ds. \end{aligned} \quad (8)$$

The results are

$$\begin{aligned} F_0'(2\eta) &= \frac{\Gamma(\frac{2}{3})}{2\sqrt{\pi}\beta^{\frac{1}{2}}} \left\{ 1 - \frac{4}{15} \frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{2}{3})} \frac{1}{\beta^2} \right. \\ &\quad \left. + \frac{272}{14175} \frac{1}{\beta^6} - \dots \right\} + \frac{1}{3\beta^3} F_0(2\eta) \\ G_0'(2\eta) &= \frac{-\sqrt{3}\Gamma(\frac{2}{3})}{2\sqrt{\pi}\beta^{\frac{1}{2}}} \left\{ 1 + \frac{4}{15} \frac{\Gamma(\frac{1}{3})}{\Gamma(\frac{2}{3})} \frac{1}{\beta^2} \right. \\ &\quad \left. + \frac{272}{14175} \frac{1}{\beta^6} - \dots \right\} + \frac{1}{3\beta^3} G_0(2\eta). \end{aligned} \quad (9)$$

For the convenience of the reader, the results in (7) and (9) are given in a form suitable for computation.

$$\begin{aligned}
 F_0(2\eta) &= 0.7063326373\eta^{1/6} \\
 &\times \left[ 1 - \frac{0.04959570165}{\eta^{4/3}} - \frac{0.00888888889}{\eta^2} - \dots \right], \\
 G_0(2\eta) &= 1.223404016\eta^{1/6} \\
 &\times \left[ 1 + \frac{0.04959570165}{\eta^{4/3}} - \frac{0.00888888889}{\eta^2} + \dots \right], \\
 F_0'(2\eta) &= \frac{0.4086957323}{\eta^{1/6}} \left[ 1 - \frac{0.6913041477}{\eta^{2/3}} \right. \\
 &\quad \left. + \frac{0.04317460317}{\eta^2} - \dots \right] + \frac{0.5}{\eta} F_0(2\eta), \\
 G_0'(2\eta) &= \frac{-0.7078817734}{\eta^{1/6}} \left[ 1 + \frac{0.6913041477}{\eta^{2/3}} \right. \\
 &\quad \left. + \frac{0.04317460317}{\eta^2} + \dots \right] + \frac{0.5}{\eta} G_0(2\eta).
 \end{aligned} \tag{10}$$

An examination of (7) and (9) shows that the expressions are useful for large values of  $\eta$ . Actually, they may be used even at  $\eta=1$  to obtain results good to a few percent.

Let us now consider the problem of determining the functional values in the neighborhood of  $\rho=2\eta$  by means of Taylor series.

To employ the Taylor expansion, one must compute the successive derivatives of  $F_0$  and  $G_0$ . Thus, if  $u=F_0$  or  $G_0$ , we have

$$\begin{aligned}
 u(\rho+\delta, \eta) &= u(\rho) + \frac{\delta}{1!} u' + \frac{\delta^2}{2!} u'' + \frac{\delta^3}{3!} u''' + \dots, \\
 u'(\rho+\delta, \eta) &= u'(\rho) + \frac{\delta}{1!} u'' + \frac{\delta^2}{2!} u''' + \frac{\delta^3}{3!} u^{iv} + \dots.
 \end{aligned} \tag{11}$$

However if we define

$$\sigma_n = \frac{\delta^n d^n u}{n! d\rho^n}, \tag{12}$$

(11) can be written

$$u(\rho+\delta, \eta) = \sum_{n=0}^{\infty} \sigma_n, \quad u'(\rho+\delta, \eta) = \delta^{-1} \sum_{n=1}^{\infty} n\sigma_n. \tag{13}$$

For hand computation the form (11) may be preferred. However, if a computer is available, (13) may be used advantageously.

The successive derivatives follow immediately from the differential equation for the Coulomb wave functions, namely,

$$\begin{aligned}
 \rho u'' + (\rho - 2\eta)u &= 0, \\
 \rho u''' + u'' + (\rho - 2\eta)u' + u &= 0, \\
 \rho u^{(n+1)} + (n-1)u^{(n)} + (\rho - 2\eta)u^{(n-1)} + (n-1)u^{(n-2)} &= 0.
 \end{aligned} \tag{14}$$

In terms of the quantities  $\sigma_n$ , (14) may be rewritten

$$\begin{aligned}
 2\rho\sigma_2 + \delta^2(\rho - 2\eta)\sigma_0 &= 0, \\
 \rho n(n+1)\sigma_{n+1} + \delta(n^2 - n)\sigma_n + \delta^2(\rho - 2\eta)\sigma_{n-1} + \delta^3\sigma_{n-2} &= 0;
 \end{aligned} \tag{15}$$

and since  $\sigma_0 = u$ ,  $\sigma_1 = \delta u'$ , one may generate as many  $\sigma_n$ 's as are needed. We note that when  $\delta$  is not small,  $u(\rho+\delta)$  may be computed in successive steps which are fractions of  $\delta$  by a procedure which is essentially a numerical integration of the differential equation starting from  $\rho=2\eta$ . We shall demonstrate the method in the case of  $u=G_0$  to obtain the value for  $\rho=6$ ,  $\eta=4$ . From Table I we have

$$G_0(8,4) = 1.5526082, \quad G_0'(8,4) = -0.5232725.$$

With the aid of (14), we get

$$\begin{aligned}
 G_0'' &= 0, & G_0^{viii} &= 0.1957515, \\
 G_0''' &= -0.1940760, & G_0^{ix} &= -0.2856133, \\
 G_0^{iv} &= 0.1793371, & G_0^x &= 0.4793638, \\
 G_0^v &= -0.0672514, & G_0^{xi} &= -0.7595047, \\
 G_0^{vi} &= 0.1306637, & G_0^{xii} &= 1.3063974, \\
 G_0^{vii} &= -0.1937505,
 \end{aligned}$$

We thus find with  $\delta=1$ ,  $G(7,4)=2.1164851$ ,  $G'(7,4)=-0.6544076$  and with  $\delta=2$ ,  $G(6,4)=3.01378$ . Starting with  $G(7,4)$  and  $G'(7,4)$  with  $\delta=1$ , we arrive at the same value for  $G(6,4)$ . The value of  $G_0(6,4)$  obtained by an independent method is 3.013787. The technique described is adapted for use with a large-scale computer. The table as given or the expressions in (10) would provide starting values for the stepwise procedure described. The recurrence relations could be used to obtain values for  $L>0$ . In applying the Taylor formula the truncating error can be controlled at each step by restricting the magnitudes of  $\delta$  and  $\sigma_n$ . The integration may be extended to the regions where the asymptotic expansion for large values of  $\rho$  or the representation in terms of Bessel-Clifford functions for large  $\eta$  may be used conveniently.