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Computer Investigation of Coulomb Wave Functions *

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Abstract. Numerical examples and heuristic reasoning are employed to illustrate the difficulties encountered in computing irregular Coulomb wave functions by Boersma's formulae.

Introduction. In the January 1969 issue of *Mathematics of Computation,* J. Boersma, [1] derives a most interesting relation between the regular and irregular Coulomb wave functions. Noting that the second-order differential equation of the Coulomb wave functions,

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

is a special case of Whittaker's equation

$$\frac{d^2w}{dz^2} + \left[-\frac{1}{4} + \frac{k}{z} + \frac{\frac{1}{4} - m^2}{z^2}\right], \qquad w = 0, \tag{2}$$

Boersma skillfully exploits the properties of the solutions $M_{k,m}(z)$, $W_{k,m}(z)$ to evolve the two following formulas.

$$\begin{aligned} G_0(\eta, \rho) = \frac{e^{2\pi\eta} - 1}{2\pi\eta}\Bigg[&\left\{\frac{1}{\rho} + 2\eta\left(\log 2\rho + \operatorname{Re}\psi(1 + i\eta) + 2\gamma - \frac{3}{2}\right)\right\} F_0(\eta, \rho) \\ &- (1 + \eta^2)^{1/2} F_1(\eta, \rho) \\ &- 4\eta \sum_{L=1}^{\infty} \frac{2L+1}{L(L+1)}(-1)^L \cos\delta_{0,L} F_L(\eta, \rho)\Bigg], \end{aligned} \tag{3}$$

$$\begin{aligned} G_1(\eta, \rho) = \frac{e^{2\pi\eta} - 1}{2\pi\eta}\Bigg[&\left\{\frac{1}{\rho^2} - \frac{2\eta}{\rho} + \frac{2}{3}(1 + 4\eta^2)\right\} \frac{F_0(\eta, \rho)}{(1 + \eta^2)^{1/2}} \\ &+ 2\eta\left\{\log 2\rho + \operatorname{Re}\psi(1 + i\eta) + 2\gamma - \frac{9}{4} - \frac{2}{3}\,\frac{1 + 4\eta^2}{1 + \eta^2}\right\} F_1(\eta, \rho) \\ &- \frac{1}{6}(4 + \eta^2)^{1/2} F_2(\eta, \rho) \\ &- 4\eta \sum_{L=1}^{\infty} \frac{2L+3}{L(L+3)}(-1)^L \cos\delta_{1,L} F_{L+1}(\eta, \rho)\Bigg], \end{aligned} \tag{4}$$

where

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$$\delta_{m,L} = \sum_{n=1}^{L} \arctan\left(\frac{\eta}{m+n}\right) + \frac{L\pi}{2}. \tag{5}$$

Since "Algorithm 292, regular Coulomb wave functions," by Walter Gautschi [2] provides accurate $F_L(\eta, \rho)$ values, and as Gautschi points out [3], the upward recursion is a trustworthy procedure for computing the irregular Coulomb wave functions, it appears that the Coulomb wave equation is numerically solvable by Boersma's technique. Unfortunately, cancellation of digits in formulas (3) and (4) is "crushing".

For the parameter ranges $\eta = 1(1)10$, $\rho = 1(1)20$ and $\eta = 11(1)20$, $\rho = 1, 2$, the results from [6] are compared with [5]. The details are displayed in Table 1. Since the behavior of G_0 and G_1 is computationally similar, only G_0 will be illustrated.

TABLE 1

Number of Digits of Agreement of Boersma's $G_0(\eta, \rho)$ with Table 14.1 of [5].

ρ \ η	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	5	5	5	5	5	5	5	5	5	4	4	3	4	3	3	2	2	1	2	1
2	5	5	5	5	4	3	2	3	3		1					ZERO				
3	5	5	5	3	2	2	1													
4	5	5	3	2																
5	5	5	3	1																
6	5	3	2																	
7	5	4	1																	
8	5	5	1																	
9	5	5	0																	
10	5	4	2																	
11	5	3	4				ZERO													
12	5	5	1																	
13	5	4	0																	
14	5	4	1																	
15	5	3	2																	
16	5	4	1																	
17	5	4	1																	
18	5	2	0																	
19	5	3	2																	
20	5	5	1																	

In [5], $\rho \doteq 1(1)20$. Therefore, for $\eta = 1(1)3$, $\rho = 21(1)40$, we produced the results of Table 2 by substituting in the Wronskian equation,

$$F_0(\eta, \rho)G_1(\eta, \rho) - F_1(\eta, \rho)G_0(\eta, \rho) = 1/(1 + \eta^2)^{1/2}.$$

A method of computing regular Coulomb wave functions, independent of Gautschi's algorithm, indicates that $F_0(\eta, \rho)$ and $F_1(\eta, \rho)$ are correct to at *least* ten floating point decimal digits. One concludes that the irregular solutions are responsible for the inaccuracies in computing the LHS of the Wronskian.

As pointed out by the referee, a rough indication of the loss of digits, q, can be obtained from

$$10^q \sim \frac{e^{2\pi\eta}}{2\pi} \times \frac{F(\eta, \rho)}{G_0(\eta, e)}.$$

The result is easily deduced from Eq. (3).

Table 2

Number of Digits of Agreement in LHS and RHS of the Wronskian Equation (see [6]).

ρ \ η	1	2	3
21	7	4	2
22	7	4	2
23	6	3	1
24	5	3	0
25	5	2	0
26	4	2	1
27	3	1	
28	3		
29	3		
30	2		
31	0		
32	2		
33	1		
34			
35		ZERO	
36			
37			
38			
39			
40			

Examples.

$$\eta = 3, \quad \rho = 5, \quad q \sim 4,$$

$$\eta = 5, \quad \rho = 5, \quad q \sim 9,$$

$$\eta = 25, \quad \rho = 10, \quad q \sim 34 \quad [4].$$

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1. J. Boersma, "Expansions for Coulomb wave functions," *Math. Comp.*, v. 23, 1969, pp. 51–59.

2. W. Gautschi, "Algorithm 292, regular Coulomb wave functions," *Comm. ACM*, v. 9, 1966, pp. 793–795.

3. W. Gautschi, "Computational aspects of three-term recurrence relations," *SIAM Rev.*, v. 9, 1967, pp. 24–82. MR **35** #3927.

4. H. F. Lutz & M. D. Karvelis, "Numerical calculation of Coulomb wave functions for repulsive Coulomb fields," *Nuclear Phys.*, v. 43, 1963, pp. 31–44.

5. M. Abramowitz, "Coulomb wave functions," in M. Abramowitz & I. A. Stegun (Editors), *Handbook of Mathematical Functions, with Formulas, Graphs and Mathematical Tables*, Nat. Bur. Standards Appl. Math. Series, 55, Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 1964; 3rd printing with corrections, 1965, Table 14.1 (5 S floating point). MR **29** #4914; MR **31** #1400.

6. Calculations performed on CDC-6600 at Lawrence Radiation Laboratory, Livermore, California (14 S floating point).