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The Zeros of Regular Coulomb Wave Functions and of Their Derivatives

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Abstract. A simple and efficient numerical method for computing the zeros of regular Coulomb wave functions and of their derivatives is presented. The method is based on the characterization of the zeros of the functions and of their derivatives in terms of eigenvalues of certain compact matrix operators. A similar approach has been reported for the computation of the zeros of Bessel functions and of their derivatives [9], [14].

1. Introduction. In [9], Grad and Zakrajsěk reported a matrix equation approach for the numerical computation of the zeros of Bessel functions $J_m(x)$ for $m \geqslant 0$. In [14], the method was further extended to include the zeros of $J_m(x)$ of any real order m and of their derivatives $J_m^{(p)}(x)$ with certain restrictions on m and p. In this paper, we shall show that the same approach is applicable for determining the zeros of regular Coulomb wave functions and of their first derivatives.

The *regular Coulomb wave function* $F_L(\eta, \rho)$ of order L, $L = 0, 1, 2, \ldots$, with a real parameter η, $-\infty < \eta < \infty$, gives one independent solution of the *Coulomb wave equation*

$$\frac{d^2w}{d\rho^2} + \left[1 - \frac{2\eta}{\rho} - \frac{L(L+1)}{\rho^2}\right] w = 0, \qquad \rho > 0, \tag{1.1}$$

which is important in nuclear physics. We shall not be concerned with the *irregular Coulomb wave function* $G_L(\eta, \rho)$, which gives a second solution of (1.1). As in the case of Bessel functions [9], [14], the method is based on the characterization of the zeros in terms of eigenvalues of certain matrix operators acting in l^2, i.e., the Hilbert space of all square-summable real sequences with norm defined by

$$\|\xi\| = \left[\sum_{n=1}^{\infty} \xi_n^2\right]^{1/2}, \qquad \xi = [\xi_1, \xi_2, \ldots]^T, \tag{1.2}$$

where the symbol T denotes the transpose operation. See Sections 2–3. A numerical method is derived and justified in Section 4. Actual numerical examples are presented in Section 5.

While numerical methods for computing the values of $F_L(\eta, \rho)$ for a given set of values, L, η, and ρ, are well known ([3]–[8], [10]–[13]), it appears that numerical methods for computing the zeros of $F_L(\eta, \rho)$ and of $dF_L(\eta, \rho)/d\rho$ for a given pair

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of L and η has not received sufficient attention. One could, of course, compute the zeros of $F_L(\eta, \rho)$ by using any one of standard root-finding methods, such as the method of bisection, the method of the false position, or the secant method, since the values of $F_L(\eta, \rho)$ can be readily computed using a standard method. However, such techniques require the advance knowledge of a fairly small interval containing a zero of the function, and moreover, the zeros of the function are found only one at a time. The method presented in this paper will obviate both of these difficulties.

For recent developments in the numerical methods for the evaluation of Coulomb wave functions, see [1]–[8], [10]–[13], and [17] and the references given there.

2. The Zeros of Regular Coulomb Wave Functions. For a given pair of numbers η and ρ, the functions $F_k(\eta, \rho)$, $k = 0, 1, 2, \ldots,$ can be characterized as a minimal solution of the linear difference equation

$$\begin{aligned}(k+2)\sqrt{(k+1)^2+\eta^2}\,u_k - (2k+3)\left[\eta + \frac{(k+1)(k+2)}{\rho}\right]u_{k+1}\\ + (k+1)\sqrt{(k+2)^2+\eta^2}\,u_{k+2} = 0.\end{aligned} \tag{2.1}$$

See [7, p. 63]. Dividing through by $\sqrt{2k+3}\,(k+1)(k+2)$ and making the definitions

$$W_k = \sqrt{2k+1}\cdot F_k(\eta, \rho), \qquad k = 0, 1, 2, \ldots, \tag{2.2}$$

$$e_k = \frac{1}{k+1}\sqrt{\frac{(k+1)^2+\eta^2}{(2k+1)(2k+3)}}, \qquad k = 0, 1, 2, \ldots, \tag{2.3}$$

$$d_k = \frac{1}{k(k+1)}, \qquad k = 1, 2, \ldots, \tag{2.4}$$

we obtain, for $k = 0, 1, 2, \ldots,$

$$e_k W_k - (\eta d_{k+1} + 1/\rho)W_{k+1} + e_{k+1}W_{k+2} = 0. \tag{2.5}$$

Writing this in matrix form for $k = L, L+1, \ldots,$ we have

$$\left(T_{L,\eta} - \frac{1}{\rho}I\right)\varphi = \psi, \tag{2.6}$$

where

$$T_{L,\eta} = \begin{bmatrix} -\eta d_{L+1} & e_{L+1} & & \mathbf{0} \\ e_{L+1} & -\eta d_{L+2} & e_{L+2} & \\ & e_{L+2} & -\eta d_{L+3} & \ddots \\ \mathbf{0} & & \ddots & \ddots \end{bmatrix} \tag{2.7}$$

which is real, symmetric and tridiagonal, and where

(2.8) $$\varphi = [W_{L+1}, W_{L+2}, \dots]^T, \qquad \psi = [-e_L W_L, 0, 0, \dots]^T.$$

By [7, Theorem 2.3, p. 35],

$$\frac{2k}{\rho}\,\frac{W_{k+1}}{W_k} = \frac{2k}{\rho}\,\frac{\sqrt{2k+3}}{\sqrt{2k+1}}\,\frac{F_{k+1}}{F_k} \longrightarrow 1 \qquad (k \longrightarrow \infty).$$

This means that the vector φ is in the space l^2. Also,

$$2k \cdot e_k \longrightarrow 1 \quad (k \longrightarrow \infty) \quad \text{and} \quad k^2 d_k \longrightarrow 1 \quad (k \longrightarrow \infty).$$

This means that the sum of the squares of all elements of $T_{L,\eta}$ is finite. Hence $T_{L,\eta}$ can be regarded as a compact operator in l^2. It is also selfadjoint (real symmetric).

THEOREM 2.1 (ZEROS OF $F_L(\eta, \rho)$). *Let L and η be given. Then $\rho \neq 0$ is a zero of $F_L(\eta, \rho)$ if and only if $1/\rho$ is an eigenvalue of $T_{L,\eta}$.*

Proof. If $\rho \neq 0$ is a zero of $F_L(\eta, \rho)$, then the vector ψ in (2.6) vanishes. Since $F_{L+1}(\eta, \rho) \neq 0$, the vector φ does not vanish. Then (2.6) implies $1/\rho$ is an eigenvalue of $T_{L,\eta}$. Conversely, let λ be a nonzero eigenvalue of $T_{L,\eta}$. We define ρ by $\lambda = 1/\rho$. Let $[\overline{W}_{L+1}, \overline{W}_{L+2}, \dots]^T \in l^2$ be an eigenvector of $T_{L,\eta}$ corresponding to λ. Define $\overline{F}_k$ for $k = L, L+1, \dots$, by

(2.9) $$\begin{cases} \overline{F}_L = 0, \\ \sqrt{2k+1}\,\overline{F}_k = \overline{W}_k, \qquad k = L+1, L+2, \dots . \end{cases}$$

Then $F_k(\eta, \rho)$ and $\overline{F}_k$ satisfy the same difference equation (2.1) for $k = L, L+1, \dots$. We have $\overline{F}_k \longrightarrow 0$ as $k \longrightarrow \infty$, since $\overline{W}_k \longrightarrow 0$ as $k \longrightarrow \infty$. This means that the $\overline{F}_k$, $k = L+1, L+2, \dots$, represent a minimal solution of (2.1). Since any pair of minimal solutions of (2.1) is linearly dependent [7, p. 25], it follows that there exists a constant $c \neq 0$ such that

(2.10) $$F_k(\eta, \rho) = c\overline{F}_k, \qquad k = L, L+1, \dots .$$

In particular, for $k = L$, $F_L(\eta, \rho) = c\overline{F}_L = 0$.

COROLLARY 2.1. *The zeros of $F_L(\eta, \rho)$ are real.*

Proof. This follows from the selfadjointness of $T_{L,\eta}$.

Remark 2.1. Consider the homogeneous equation

(2.11) $$T_{L,\eta}\varphi = 0.$$

Writing $\varphi = [W_{L+1}, W_{L+2}, \dots]^T$, this is equivalent to

(2.12) $$\begin{aligned} -\eta d_{L+1} W_{L+1} + e_{L+1} W_{L+2} &= 0, \\ e_k W_k - \eta d_{k+1} W_{k+1} + e_{k+1} W_{k+2} &= 0, \qquad k \geq L+1. \end{aligned}$$

Assume $\eta \neq 0$. Then (see, e.g., [7, pp. 34–35]), there exists an independent solution of (2.12) such that

$$\frac{e_k}{\eta d_k} \cdot \frac{W_{k+1}}{W_k} \longrightarrow 1 \quad \text{as } k \longrightarrow \infty,$$

i.e.,

$$\frac{k}{\eta}\frac{W_{k+1}}{W_k} \longrightarrow 2 \quad \text{as } k \longrightarrow \infty.$$

This shows that, *if* $\eta \neq 0$, *then* (2.11) *has a nontrivial solution in* l^2. If $\eta = 0$, then (2.11) reduces to

$$\begin{cases} W_{L+2} = 0, \\ e_k W_k + e_{k+1} W_{k+2} = 0, \qquad k \geqslant L+1. \end{cases} \tag{2.13}$$

It follows that (2.11) has only the trivial solution in l^2 if $\eta = 0$, since $e_k > e_{k+1}$.

Remark 2.2. Let $D = \operatorname{diag}[-1, 1, -1, 1, \ldots]$. Then $D^2 = I$ and

$$D(-T_{L,\eta})D = \begin{bmatrix} \eta d_{L+1} & e_{L+1} & & \mathbf{0} \\ e_{L+1} & \eta d_{L+2} & e_{L+2} & \\ & e_{L+2} & \eta d_{L+3} & \ddots \\ \mathbf{0} & & \ddots & \ddots \end{bmatrix} = T_{L,-\eta}. \tag{2.14}$$

This shows that $-T_{L,\eta}$ is similar to $T_{L,-\eta}$. Consequently, *the positive zeros of* $F_L(-\eta, \rho)$ *are given precisely by the absolute values of the negative zeros of* $F_L(\eta, \rho)$. Hence, by solving an eigenvalue problem (2.6), the positive zeros of $F_L(\eta, \rho)$ and of $F_L(-\eta, \rho)$ are computed simultaneously.

Remark 2.3. If $\eta = 0$, then

$$F_L(\eta, \rho) = F_L(0, \rho) = \sqrt{\frac{\pi}{2}\cdot\rho}\, J_{L+(1/2)}(\rho).$$

Hence, the positive zeros of $F_L(0, \eta)$ are identical with those of $J_{L+(1/2)}(\rho)$, i.e., the Bessel function of order $L + (1/2)$. In particular, for $L = \eta = 0$,

$$F_0(0, \rho) = \sqrt{\frac{\pi}{2}\rho}\, J_{1/2}(\rho) = \sin\rho.$$

3. The Zeros of the First Derivative of Regular Coulomb Wave Functions. We retain the notation used in Section 2. It is known that, for $L = 0, 1, 2, \ldots,$

$$(L+1)\frac{dF_L}{d\rho} = \left[\frac{(L+1)^2}{\rho} + \eta\right] F_L - \sqrt{(L+1)^2 + \eta^2}\, F_{L+1}. \tag{3.1}$$

Hence, $dF_L/d\rho = 0$ if and only if

$$\left[\frac{(L+1)^2}{\rho} + \eta\right] F_L - \sqrt{(L+1)^2 + \eta^2}\, F_{L+1} = 0. \tag{3.2}$$

This can be written as

$$-\left[\frac{\eta}{(L+1)^2} + \frac{1}{\rho}\right]\sqrt{\frac{L+1}{2L+1}}\, W_L + \sqrt{\frac{2L+1}{L+1}}\, e_L W_{L+1} = 0. \tag{3.3}$$

If we consider (3.3) together with the difference equation (2.5), we obtain the following matrix equation

$$\left(\widetilde{T}_{L,\eta} - \frac{1}{\rho} I\right)\widetilde{\varphi} = 0, \tag{3.4}$$

where

$$\widetilde{T}_{L,\eta} = \begin{bmatrix} -\frac{\eta}{(L+1)^2} & \sqrt{\frac{2L+1}{L+1}}\, e_L & & & \mathbf{0} \\ \sqrt{\frac{2L+1}{L+1}}\, e_L & -\eta d_{L+1} & e_{L+1} & & \\ & e_{L+1} & -\eta d_{L+2} & e_{L+2} & \\ \mathbf{0} & & e_{L+2} & \ddots & \ddots \\ & & & \ddots & \ddots \end{bmatrix} \tag{3.5}$$

which is real, symmetric, and tridiagonal, and where

$$\widetilde{\varphi} = \left[\sqrt{\frac{L+1}{2L+1}}\, W_L, W_{L+1}, W_{L+2}, \ldots\right]^T. \tag{3.6}$$

Just like $T_{L,\eta}$ in Section 2, $\widetilde{T}_{L,\eta}$ is a compact operator in l^2.

THEOREM 3.1 (ZEROS OF $dF_L/d\rho$). *Let L and η be given. Then $\rho \neq 0$ is a zero of $dF_L(\eta, \rho)/d\rho$ if and only if $1/\rho$ is an eigenvalue of $\widetilde{T}_{L,\eta}$.*

The proof is similar to that of Theorem 2.1 and is omitted.

COROLLARY 3.1. *The zeros of $dF_L/d\rho$ are real.*

Remark 3.1. As for $T_{L,\eta}$, 0 is an eigenvalue of $\widetilde{T}_{L,\eta}$ when $\eta \neq 0$, and is not when $\eta = 0$.

Remark 3.2. The positive zeros of $dF_L(-\eta, \rho)/d\rho$ are given precisely by the absolute values of the negative zeros of $dF_L(\eta, \rho)/d\rho$. See Remark 2.2.

4. The Numerical Procedure. A numerical method for computing the zeros of $F_L(\eta, \rho)$ and of $dF_L(\eta, \rho)/d\rho$ for a given pair of numbers L and η is now presented.

(I) *Zeros of $F_L(\eta, \rho)$*. Let n be a positive integer. Let $T^{(n)}_{L,\eta}$ denote the principal $n \times n$ submatrix of $T_{L,\eta}$. We shall refer to $T^{(n)}_{L,\eta}$ as the *truncated matrix of order n*. It is known that the nonvanishing zeros of $F_L(\eta, \rho)$ are simple. Hence, by Theorem 2.1, all nonzero eigenvalues of $T_{L,\eta}$ are simple. By the Sturm-sequence theorem [16, pp. 299–302], the eigenvalues of $T^{(n)}_{L,\eta}$ are also simple. Let $\lambda_{-1} < \lambda_{-2} < \ldots < 0 < \ldots < \lambda_2 < \lambda_1$ be a complete enumeration of the nonzero eigenvalues of $T_{L,\eta}$. Let $\lambda^{(n)}_{-1} < \lambda^{(n)}_{-2} < \ldots < 0 < \ldots < \lambda^{(n)}_2 < \lambda^{(n)}_1$ be a complete enumeration of the eigenvalues of $T^{(n)}_{L,\eta}$. The zeros of $F_L(\eta, \rho)$ are approximated by $1/\lambda^{(n)}_k$, where $\lambda^{(n)}_k \neq 0$. By [13, pp. 279–281], we have the following estimate for any k:

$$|\lambda^{(n)}_k - \lambda_k| \leq \|T^{(n)}_{L,\eta} - T_{L,\eta}\| \quad \text{(operator norm)}.$$

TABLE 1

The least 5 positive zeros of $F_L(\eta, \rho)$ correct to 10 figures

L = 0					
η = 0		η = 1		η = 2	
3.1415 92654	(00)	5.8141 15616	(00)	8.3956 70124	(00)
6.2831 85307	(00)	9.4745 33918	(00)	1.2405 24258	(01)
9.4247 77961	(00)	1.2941 65270	(01)	1.6110 44740	(01)
1.2566 37061	(01)	1.6323 24836	(01)	1.9676 31893	(01)
1.5707 96327	(01)	1.9655 75668	(01)	2.3160 32851	(01)
η = 4		η = 8		η = 16	
1.3219 26777	(01)	2.2323 33111	(01)	3.9766 16365	(01)
1.7742 90736	(01)	2.7571 88361	(01)	4.6002 24064	(01)
2.1815 35538	(01)	3.2182 80961	(01)	5.1369 31880	(01)
2.5674 09274	(01)	3.6482 71962	(01)	5.6302 69889	(01)
2.9404 17556	(01)	4.0591 23272	(01)	6.0964 36277	(01)
L = 1					
η = 0		η = 1		η = 2	
4.4934 09458	(00)	6.5665 70904	(00)	8.8510 65605	(00)
7.7252 51837	(00)	1.0238 85720	(01)	1.2863 21977	(01)
1.0904 12166	(01)	1.3711 33324	(01)	1.6569 69608	(01)
1.4066 19391	(01)	1.7096 05052	(01)	2.0136 34835	(01)
1.7220 75527	(01)	2.0430 62027	(01)	2.3620 89262	(01)
η = 4		η = 8		η = 16	
1.3462 75189	(01)	2.2447 45611	(01)	3.9828 54985	(01)
1.7986 76787	(01)	2.7696 05220	(01)	4.6064 63125	(01)
2.2059 42254	(01)	3.2307 00483	(01)	5.1431 71234	(01)
2.5918 29573	(01)	3.6606 93361	(01)	5.6365 09465	(01)
2.9648 47623	(01)	4.0715 46094	(01)	6.1026 76029	(01)

The bound on the right-hand side of the last inequality converges to 0 as $n \longrightarrow \infty$, but the bound is usually too pessimistic. In practice, it is enough to observe the numerical convergence $\lambda_k^{(n)} \longrightarrow \lambda_k$.

(II) A similar procedure applies in the numerical computation of the zeros of $dF_L(\eta, \rho)/d\rho$. Thus, if $\widetilde{T}_{L,\eta}^{(n)}$ denotes the principal $n \times n$ submatrix of $\widetilde{T}_{L,\eta}$, then the zeros of $F_L(\eta, \rho)$ are approximated by $1/\widetilde{\lambda}_k^{(n)}$, where $\widetilde{\lambda}_k^{(n)}$ represents an arbitrary non-vanishing eigenvalue of $\widetilde{T}_{L,\eta}^{(n)}$.

TABLE 2

The least 5 positive zeros of $dF_L(\eta, \rho)/d\rho$ correct to 10 figures

L = 0					
$\eta = 0$		$\eta = 1$		$\eta = 2$	
1.5707 96327	(00)	3.6574 10638	(00)	5.8950 85350	(00)
4.7123 88980	(00)	7.6676 77779	(00)	1.0436 57415	(01)
7.8539 81634	(00)	1.1216 79693	(01)	1.4271 84702	(01)
1.0995 57429	(01)	1.4637 06308	(01)	1.7901 00351	(01)
1.4137 16694	(01)	1.7992 37821	(01)	2.1423,16801	(01)
$\eta = 4$		$\eta = 8$		$\eta = 16$	
1.0250 63372	(01)	1.8732 88298	(01)	3.5364 34308	(01)
1.5533 79997	(01)	2.5020 84729	(01)	4.2982 88977	(01)
1.9800 33171	(01)	2.9907 84803	(01)	4.8727 92458	(01)
2.3756 58102	(01)	3.4350 24172	(01)	5.3860 63072	(01)
2.7546 82974	(01)	3.8548 53936	(01)	5.8650 08314	(01)
L = 1					
$\eta = 0$		$\eta = 1$		$\eta = 2$	
2.7437 07270	(00)	4.3875 03851	(00)	6.3463 01319	(00)
6.1167 64264	(00)	8.4269 47553	(00)	1.0893 42998	(01)
9.3166 15629	(00)	1.1984 04802	(01)	1.4730 51307	(01)
1.2485 93737	(01)	1.5408 41197	(01)	1.8360 66699	(01)
1.5643 86611	(01)	1.8766 26782	(01)	2.1883 47826	(01)
$\eta = 4$		$\eta = 8$		$\eta = 16$	
1.0493 61433	(01)	1.8856 95887	(01)	3.5426 72491	(01)
1.5777 38308	(01)	2.5144 99607	(01)	4.3045 27833	(01)
2.0044 30293	(01)	3.0032 03073	(01)	4.8790 21673	(01)
2.4000 71979	(01)	3.4474 44675	(01)	5.3923 02541	(01)
2.7791 08373	(01)	3.8672 76073	(01)	5.8712 47981	(01)

5. Examples. Some of our computational results follow.

Tables 1 and 2 show the first five positive zeros of $F_L(\eta, \rho)$ and of $dF_L(\eta, \rho)/d\rho$ correct to 10 decimal figures, for $L = 0$ and 1 and $\eta = 0, 1, 2, 4, 8$, and 16. In practical applications of the regular Coulomb wave functions, η is usually positive.

Table 3 shows the first positive zeros of $F_L(\eta, \rho)$ and of $dF_L(\eta, \rho)/d\rho$ correct to 10 decimal figures for $L = 1$ and $\eta = -1$, as an example of the case of negative η. This requires no new computations as stated in Remark 2.2.

TABLE 3

The least 5 positive zeros of $F_1(-1, \rho)$ and of $dF_1(-1, \rho)/d\rho$, correct to 10 figures

$F_1(-1,\rho)$		$dF_1(-1,\rho)/d\rho$	
2.9661 44623	(00)	1.6804 42277	(00)
5.6619 20828	(00)	4.3025 20276	(00)
8.4788 75692	(00)	7.0635 49724	(00)
1.1368 94161	(01)	9.9196 30533	(00)
1.4306 33125	(01)	1.2834 75614	(01)

TABLE 4

The number of computed positive zeros of $F_L(\eta, \rho)$ correct to 10 or more figures

η	L = 0			L = 1		
	n = 32	n = 64	n = 128	n = 32	n = 64	n = 128
16	0	5	21	0	5	21
8	1	8	26	1	9	26
4	3	11	29	3	11	29
2	4	13	31	4	13	31
1	5	14	33	5	14	32
0	6	15	34	6	15	34
-1	7	16	36	7	15	35
-2	8	17	37	7	17	37
-4	9	19	39	8	19	39
-8	11	22	43	10	21	42
-16	13	25	47	12	24	47

TABLE 5

The number of computed positive zeros of $dF_L(\eta, \rho)/d\rho$ correct to 10 or more figures

η	L = 0			L = 1		
	n = 32	n = 64	n = 128	n = 32	n = 64	n = 128
16	0	5	21	0	5	21
8	2	9	26	2	9	26
4	3	11	30	3	11	30
2	4	12	32	5	12	32
1	5	14	33	5	14	33
0	6	15	35	6	15	34
-1	7	17	36	7	16	36
-2	8	18	37	8	17	37
-4	9	19	40	9	19	39
-8	11	22	43	11	21	42
-16	13	25	48	12	25	47

Tables 4 and 5 show how the number of computed positive zeros of $F_L(\eta, \rho)$ and of $dF_L(\eta, \rho)/d\rho$, correct to 10 or more figures, depends on L, η, and n, where n denotes the order of the truncated matrices $T^{(n)}_{L,\eta}$ or $\widetilde{T}^{(n)}_{L,\eta}$ (see Section 4). For instance, Table 4 indicates that for $L = 1$ and $\eta = 1$ the use of the truncated matrix of order $n = 64$ produces the *first* 14 positive zeros of $F_L(\eta, \rho)$, correct to 10 or more significant figures. The number was determined by comparing the computed zeros for successive values of n.

The computations were done on the CDC 6600/6400 system at The University of Texas at Austin, using single-precision (net 48-bit) floating-point arithmetic (FORTRAN REAL arithmetic). For the computation of the eigenvalues of real symmetric tridiagonal matrices, the FORTRAN subroutine IMTQLI in EISPACK [16] was used. The computing time (the CDC 6600 central processor time) depends on n. About 0.86 seconds were needed for $n = 64$, 2.0 seconds for $n = 128$, and 6.6 seconds for $n = 256$.

Note. In the above tables, the numbers appearing in parentheses represent the exponent relative to base 10. For instance, 1.321926777 (01), i.e., the first positive zero of $F_L(\eta, \rho)$ for $L = 0$ and $\eta = 4$ (Table 1), means 1.321926777×10^1.

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