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Chebyshev Approximations for the Coulomb Phase Shift*

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Abstract. This note presents nearly-best rational approximations for the Coulomb phase shift $\sigma_0(\eta) = \arg \Gamma(1 + i\eta)$. Maximal relative errors range down to between 4.24×10^{-19} and 1.09×10^{-20}. The nontrivial zero of $\sigma_0(\eta)$ is also given.

1. Introduction. The Coulomb wave functions $F_L(\eta, \rho)$ and $G_L(\eta, \rho)$ are the two real, linearly independent solutions of the second-order differential equation

$$d^2y/d\rho^2 + [1 - 2\eta/\rho - L(L + 1)/\rho^2]y = 0$$

that have the asymptotic behavior for large ρ

$$F_L(\eta, \rho) \sim \sin\left(\rho - \eta \ln 2\rho - \frac{L}{2}\pi + \sigma_L(\eta)\right)$$

and

$$G_L(\eta, \rho) \sim \cos\left(\rho - \eta \ln 2\rho - \frac{L}{2}\pi + \sigma_L(\eta)\right),$$

where the quantity

$$\sigma_L(\eta) = \arg \Gamma(L + 1 + i\eta) = \operatorname{Im} \{\ln \Gamma(L + 1 + i\eta)\}$$

is the Coulomb phase shift [1]. These Coulomb functions and phase shifts are frequently of importance in quantum-mechanical scattering problems.

At present, satisfactory techniques exist for calculation of the $F_L(\eta, \rho)$ [2], [3], but the techniques for calculating the $G_L(\eta, \rho)$ and the $\sigma_L(\eta)$ [4], [5] are slow and not too accurate. In particular, calculation of the $\sigma_L(\eta)$ is generally based on the asymptotic expansion of $\ln \Gamma(z)$. Using the first three terms in this expansion, we find

$$\begin{aligned}\sigma_{L-1}(\eta) \simeq& -\eta + \frac{\eta}{2} \ln (L^2 + \eta^2) + \frac{2L - 1}{2} \arctan (\eta/L) \\ &+ \frac{-\eta}{12(L^2 + \eta^2)}\left[1 + \frac{\eta^2 - 3L^2}{30(L^2 + \eta^2)^2} + \frac{\eta^4 - 10L^2\eta^2 + 5L^4}{105(L^2 + \eta^2)^4}\right].\end{aligned} \tag{1.1}$$

Lutz and Karvelis [4] use this approximation for $L = 4$, and then calculate $\sigma_0(\eta)$, as well as $\sigma_L(\eta)$ for other L, from the relation

$$\sigma_0(\eta) = \sigma_L(\eta) - \sum_{j=1}^{L} \arctan (\eta/j). \tag{1.2}$$

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TABLE I. $E_{lm} = -100 \log_{10} \max_{\eta} \left| \frac{\sigma_0(\eta) - \tilde{\sigma}_{lm}(\eta)}{\sigma_0(\eta)} \right|$

$|\eta| \leqq 2.0$

	l									
m	0	1	2	3	4	5	6	7	8	9
0		106	160	211	261					
1	155	244	322	393	459					
2	223	355	449*	531	607					
3	283	438	554	648	736					
4	338	511	641	754	851*					
5						1050				
6							1252*			
7								1453		
8									1653*	
9										1854*

$2.0 \leqq \eta \leqq 4.0$

m	0	1	2	3	4	5	6	7	8	9
0		83	152	217	279	339				
1		211	310	396	475					
2		295	431*	535						
3		368	527	654						
4		436	613		879*					
5						1101*				
6							1324			
7								1550		
8									1772*	
9										1996*

$4.0 \leqq \eta$

m	0	1	2	3	4	5	6	7	8	9
0		448	636	828	1015	1215				
1	445	717*	934	1110	1263					
2	628	935	1094	1307	1392					
3	815	1109	1311	1391*	1470					
4	998	1263	1392	1467	1545					
5						1710*				
6							1837*			

* Coefficients for these approximations only are given in Tables II—IV.

In this note we present rational Chebyshev approximations that allow rapid, direct evaluation of $\sigma_0(\eta)$ for up to 20 significant decimal places. Equation (1.2) can then be used to find $\sigma_L(\eta)$ for other L. In addition, the nontrivial zero of $\sigma_0(\eta)$ is presented to 22 decimal places.

2. Generation of the Approximations. The forms of the approximations and the values of η for which they are used are

$$\sigma_0(\eta) \simeq \eta(\eta^2 - \eta_0^2)R_{lm}(\eta^2), \qquad 0 \leqq \eta \leqq 2.0,$$

$$\simeq \eta R_{lm}(\eta^2), \qquad 2.0 \leqq \eta \leqq 4.0,$$

$$\simeq \frac{\arctan(\eta)}{2} + \eta\left[\frac{\ln(1+\eta^2)}{2} + R_{lm}(1/\eta^2)\right], \qquad 4.0 \leqq \eta,$$

where

$$\eta_0 = 1.80554\ 70716\ 05106\ 91987\ 64$$

is the positive nontrivial zero of $\sigma_0(\eta)$, and the $R_{lm}(z)$ are rational functions of degree l in the numerator and m in the denominator.

Standard versions of the Remes algorithm for rational Chebyshev approximation [6], [7] were used to generate the rational approximations. Function values were computed as needed using various methods, depending on the value of η. For small η, the computation was based on the series expansion

$$\text{(2.1)} \quad \ln \Gamma(1+z) = -\ln(1+z) + z(1-\gamma) + \sum_{n=2}^{\infty} (-1)^n[\zeta(n) - 1]\frac{z^n}{n}, \quad |z| < 2.$$

The power series for $\sigma_0(\eta)$ derived from (2.1) was transformed into a rapidly convergent and computationally stable continued fraction. Necessary values of $\zeta(n) - 1$ were computed to an accuracy of 25S with 40S arithmetic.

For $|\eta - \eta_0| < .0005$, a Taylor's series expansion about η_0 was used. For all other values of η, $\sigma_0(\eta)$ was computed by first using the well-known convergent continued fraction to evaluate $\ln \Gamma(5 + i\eta)$, and then recurrence (1.2). Newton's method was used to determine η_0.

All computations were carried out on a CDC-3600 computer in 25S arithmetic. By comparing the various methods for computing $\sigma_0(\eta)$ against one another, the accuracy of the master routines was verified to at least 22S.

3. Results. Table I lists the values of

$$E_{lm} = -100 \log_{10} \max_{\eta} \left|\frac{\sigma_0(\eta) - \tilde{\sigma}_{lm}(\eta)}{\sigma_0(\eta)}\right|,$$

(here $\tilde{\sigma}_{lm}(\eta)$ denotes the appropriate approximation and the maximum is taken over the appropriate interval) for the initial segments of the various L_∞ Walsh arrays. Tables II–IV present coefficients for selected approximations along the main diagonals of these arrays.

All coefficients are given to an accuracy slightly greater than that justified by the maximal errors, but reasonable additional rounding should not seriously affect

TABLE II. $\sigma_0(\eta) \simeq \sigma_{nn}(\eta) = \eta(\eta^2 - \eta_0^2) \sum_{j=0}^{n} p_j\eta^{2j} \Big/ \sum_{j=0}^{n} q_j\eta^{2j}$ $|\eta| \leq 2.0$

n	j	p_j		q_j	
2	0	1.46897 5	(00)	8.29675 4	(00)
	1	7.36858 7	(−01)	7.36816 8	(00)
	2	1.83678 8	(−02)	1.00000 0	(00)
4	0	2.89400 39291	(01)	1.63447 63441	(02)
	1	3.82797 75977	(01)	2.79519 66647	(02)
	2	1.36400 64026	(01)	1.46028 79586	(02)
	3	1.19614 84185	(00)	2.48513 50161	(01)
	4	7.14117 04272	(−03)	1.00000 00000	(00)
6	0	7.26231 75420 0794	(02)	4.10161 37088 4059	(03)
	1	1.54822 08152 6481	(03)	1.03330 98198 2759	(04)
	2	1.14884 20205 4676	(03)	9.50548 18490 6670	(03)
	3	3.54878 61514 8409	(02)	3.92344 52839 1116	(03)
	4	4.28515 43392 7621	(01)	7.23157 75777 8917	(02)
	5	1.51185 53281 8749	(00)	5.20817 64819 7408	(01)
	6	3.78421 31532 1365	(−03)	1.00000 00000 0000	(00)
8	0	2.01061 42480 06387 007	(04)	1.13555 52707 66994 359	(05)
	1	5.91099 15291 67068 016	(04)	3.77834 96966 76579 556	(05)
	2	6.72663 08978 48372 087	(04)	4.98984 26839 98281 159	(05)
	3	3.75299 23373 45015 120	(04)	3.34393 60399 70151 738	(05)
	4	1.07511 39163 93479 392	(04)	1.20938 93155 30544 191	(05)
	5	1.51702 27985 59215 518	(03)	2.32936 00087 64246 542	(04)
	6	9.23457 41447 74635 177	(01)	2.21972 74313 37920 938	(03)
	7	1.75100 14594 87020 923	(00)	8.87380 35740 41218 697	(01)
	8	2.34438 18744 24005 593	(−03)	1.00000 00000 00000 000	(00)
9	0	1.08871 50490 47974 11683	(05)	6.14884 78634 60711 35090	(05)
	1	3.64707 57308 11609 14640	(05)	2.29801 58851 57080 14282	(06)
	2	4.88801 47158 28780 13158	(05)	3.50310 84412 84240 21934	(06)
	3	3.36275 73629 81973 24009	(05)	2.81194 99028 60410 80264	(06)
	4	1.26899 22627 78384 79804	(05)	1.28236 44199 43584 06742	(06)
	5	2.60795 54352 70845 82682	(04)	3.35209 34871 18037 53154	(05)
	6	2.73352 48055 44979 90544	(03)	4.84319 58024 79487 01171	(04)
	7	1.26447 54356 99029 63184	(02)	3.54877 03900 68732 06531	(03)
	8	1.85446 02212 55339 09390	(00)	1.11207 20129 98043 90166	(02)
	9	1.90716 21999 00376 48146	(−03)	1.00000 00000 00000 00000	(00)

the accuracy of the approximations. All approximations listed were checked by comparing computations with the coefficients as they are presented here against computations with the master function routines.

With a little care, accurate computer subroutines that use these approximations can be written. For $0 \leqq \eta \leqq 2.0$, the computation of the factor $\eta^2 - \eta_0^2$ is critical

TABLE III. $\sigma_0(\eta) \simeq \tilde{\sigma}_{nn}(\eta) = \eta \sum_{j=0}^{n} p_j \eta^{2j} \Big/ \sum_{j=0}^{n} q_j \eta^{2j}$ $\quad 2.0 \leqq \eta \leqq 4.0$

n	j	p_j		q_j	
2	0	−6.15755 9	(01)	1.18922 3	(02)
	1	1.34835 8	(01)	3.92749 5	(01)
	2	1.66075 1	(00)	1.00000 0	(00)
4	0	−1.30199 63766	(04)	2.27000 07374	(04)
	1	−2.58467 97911	(03)	1.98507 22472	(04)
	2	1.44516 43973	(03)	3.68942 31707	(03)
	3	1.68405 20098	(02)	1.57437 62626	(02)
	4	2.23854 04975	(00)	1.00000 00000	(00)
5	0	−1.96332 77985 787	(05)	3.40681 78321 482	(05)
	1	−8.50114 05797 202	(04)	3.82020 31307 722	(05)
	3	6.55460 31287 939	(03)	9.98364 41488 102	(03)
	4	3.17745 47883 836	(02)	2.44870 49151 213	(02)
	5	2.43456 50037 542	(00)	1.00000 00000 000	(00)
8	0	−6.85617 78344 55812 7516	(08)	1.18783 00450 03677 0748	(09)
	1	−8.13831 98338 42941 1218	(08)	2.23434 70745 46813 1611	(09)
	2	−1.89579 59754 89882 1821	(08)	1.45302 53317 43155 6033	(09)
	3	5.27771 80138 86035 8173	(07)	4.10263 69336 99893 9991	(08)
	4	2.24410 15897 37091 5014	(07)	5.32475 62681 40404 6468	(07)
	5	2.38405 47089 67944 6349	(06)	3.12188 92522 01429 6487	(06)
	6	9.01065 75392 98215 0217	(04)	7.58778 58146 97289 8291	(04)
	7	1.10783 80003 39040 0140	(03)	6.23847 23297 51985 3161	(02)
	8	2.86371 39999 87846 4927	(00)	1.00000 00000 00000 0000	(00)
9	0	−1.04410 09875 26487 61867 0	(10)	1.80886 81614 93543 88778 7	(10)
	1	−1.50857 41071 80079 91369 6	(10)	3.86914 20517 04700 26778 5	(10)
	2	−5.58265 28333 55901 16054 2	(09)	3.00326 45751 47162 63404 6	(10)
	3	4.05252 91743 69477 27544 6	(08)	1.07555 46514 94601 84352 5	(10)
	4	5.46171 22731 18594 27519 2	(08)	1.90129 85018 23290 69424 5	(09)
	5	9.51040 44030 68169 39571 4	(07)	1.66599 98321 51229 47263 2	(08)
	6	6.28112 66099 97342 11941 6	(06)	6.95218 80891 69487 37593 6	(06)
	7	1.65117 80489 50518 52041 6	(05)	1.25323 50806 25688 65271 8	(05)
	8	1.49882 44213 29341 28552 1	(03)	7.90442 04145 60291 39699 6	(02)
	9	2.97468 65065 95477 98477 6	(00)	1.00000 00000 00000 00000 0	(00)

TABLE IV. $\sigma_0(\eta) \simeq \sigma_{nn}(\eta) = \dfrac{\arctan(\eta)}{2} + \eta\left[\dfrac{\ln(1+\eta^2)}{2} + \sum_{j=0}^{n} p_j\eta^{-2j} \Big/ \sum_{j=0}^{n} q_j\eta^{-2j}\right]$

$4.0 \leqq \eta$

n	j	p_j		q_j	
1	0	−1.02049 5193	(00)	1.02049 5395	(00)
	1	−1.08507 3052	(00)	1.00000 0000	(00)
3	0	5.52387 17153 35895	(00)	−5.52387 17153 35634	(00)
	1	−3.36547 45149 49993	(00)	3.82579 71576 79412	(00)
	2	−8.63325 41266 93300	(00)	7.86945 91836 37064	(00)
	3	−9.74960 20678 93389	(−01)	1.00000 00000 00000	(00)
5	0	−1.02229 38942 37776 1129	(00)	1.02229 38942 37776 0774	(00)
	1	1.29843 55616 25569 2388	(01)	−1.30695 46774 10877 4453	(01)
	2	−7.46013 37176 85084 4902	(01)	7.57728 17527 25597 9398	(01)
	3	−2.43096 53671 40429 7045	(−01)	−7.19309 37904 99242 8240	(00)
	4	7.02512 19333 38481 8601	(01)	−6.26120 40940 73034 9169	(01)
	5	−2.21207 38212 47507 1983	(00)	1.00000 00000 00000 0000	(00)
6	0	7.08638 61102 45209 06826	(−03)	−7.08638 61102 45209 08189	(−03)
	1	−6.54026 36894 78015 91128	(−02)	6.59931 69070 63396 30254	(−02)
	2	2.92684 14310 61580 43933	(−01)	−2.98754 42163 20586 18922	(−01)
	3	4.66821 39231 96656 09167	(00)	−4.63752 35551 34122 48006	(00)
	4	−3.43943 79038 26909 49054	(00)	3.79700 45409 88635 41593	(00)
	5	−7.72786 48686 92529 94370	(00)	7.06184 06542 63367 18524	(00)
	6	−9.88841 77120 02906 47461	(−01)	1.00000 00000 00000 00000	(00)

when $\eta \simeq \eta_0$ if one is to maintain essential machine precision in the function value. It is best to compute $\eta^2 - \eta_0^2$ as $(\eta - \eta_0)(\eta + \eta_0)$, with the factor $\eta - \eta_0$ computed to higher than machine precision. This can be accomplished by representing η_0 in two parts, $\eta_0 \equiv \eta_1 + \eta_2$, such that the floating point exponent for η_2 is much less than that for η_1. To facilitate that representation, we give both the octal and hexadecimal representation of η_0:

$$\eta_0 = 1.63434\ 12515\ 76727\ 04710\ 44565_8$$

$$= 1.\mathrm{CE385}\ 537\mathrm{EE}\ \mathrm{B89C8}\ 92\mathrm{EA}_{16}.$$

Then $(\eta - \eta_0)$ may be computed accurately as $(\eta - \eta_0) = (\eta - \eta_1) - \eta_2$.

In addition, in at least one case the conditioning of an approximation in the interval $2.0 \leqq \eta \leqq 4.0$ was improved by evaluating it in the form

$$\eta \sum_{j=0}^{n} p_{n-j}\eta^{-2j} \Big/ \sum_{j=0}^{n} q_{n-j}\eta^{-2j}$$

by use of nested multiplication.

If function values are desired for negative arguments, the relation

$$\sigma_0(-\eta) = -\sigma_0(\eta)$$

can be used.

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