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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

ON THE ANALYTIC CONTINUATION OF FUNCTIONS DEFINED BY LEGENDRE SERIES *

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ABSTRACT

An infinite diagonal sequence of Punctual Padé Approximants is considered for the approximate analytical continuation of a function defined by a formal Legendre series. The technique is tested in the case of two series with exactly known analytical sum: the generating function for Legendre polynomials and the Couldmbian scattering amplitude.

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I. INTRODUCTION

Given a formal Legendre series

$$f(z) = \sum_{n=0}^{\infty} a_n P_n(z) \ , \qquad (1.1)$$

such that

$$\lim_{n\to\infty} \sup |a_n|^{\frac{1}{n}} = R^{-1}$$

with $R > 1$, the series is known to converge within the interior of an elliptical domain in the z-plane, with foci at $z = \pm 1$ and such that the sum of its axis is R [1] . When R = 1 that region collapses to the segment [-1,1] and the convergence is restricted, in principle, to within that segment.

The problem of summation of such an expansion is of great interest in many physical applications where the solution of the problems under study can be formally expressed as such a series. Two problems are the typical ones of interest:

i) To find a way of accelerating the convergence of (1.1) when it is slowly convergent, or even regularizing it when non-convergent, in the physical interval [-1,1];

ii) To find a way of performing the analytical continuation of f(z) in the z-plane, starting from the information contained in the terms of the series, and out of the interval [-1,1].

These problems have motivated the development of several summation techniques within the Padé-type rational approximation framework [2-6], mainly intended for their application in potential scattering calculations. Of particular interest is the Punctual Padé Approximant (PPA) method [3]. This approach is related to a non-linear sequence transformation introduced by Shanks [7] and, as briefly discussed in Sec.II, to ordinary Padé approximants (PA's) evaluated at a particular point. Moreover, it has the attractive feature, from the numerical point of view, of counting on algorithms such as Wynn's Epsilon and Bauer's Eta algorithms [8], which allow for the recurrent calculation of successive approximations.

Having in mind problem i), the convergence of the PPA's was proven within the domains where the original series is convergent, and also in situations when it is non-convergent, restricted to the cases in which f(z) can be expected to be finite, for $z \in [-1,1]$ [3-5].

The rational nature of the approximations, however, allow us also to expect them to be a valuable means for the approximate solution to problem ii). The previous proofs, dealt with the row sequences of the Padé table. Numerical studies showed that these sequences break down out of the natural domains where the series converge, i.e. elliptical regions or the interval [-1,1] [9] suggesting that diagonal-type sequences of PPA's should be considered for problems of type ii). The convergence properties of this type of sequences depend on global features of the coefficients $\{a_n\}$, whereas that of the row sequences depend only on their asymptotic behaviour. Because of this, it is very difficult, in general, to prove formal results for diagonal PPA's. An insight of what can be expected regarding their convergence can be however obtained by considering the case of a particular f(z), the generating function for Legendre polynomials and its associated series expansion, which we do in Sec.III. In this case, we are able to prove that the domain of convergence of an infinite sequence of diagonal PPA's is that of analyticity of the function. Moreover, a numerical study shows, in particular, the practical value of the sequence when approximating the correct analytical continuation of f(z). This is also verified in the case of the Coulombian scattering amplitude which we discuss in Sec.IV, suggesting that we may expect the method to be effective for more general types of Legendre series.

II. THE PPA METHOD

Associated to f(z) given by Eq.(1.1) we may define

$$F(z,x) = \sum_{n=0}^{\infty} a_n P_n(z)\, x^n = \sum_{n=0}^{\infty} c_n x^n , \tag{2.1}$$

and define the Padé Approximant (PA) $[M,N]_F$ [10] to the power series in x (and for fixed z), as

$$[M,N]_{F(z,x)} = \frac{r_0 + r_1 x + \dots + r_N x^N}{1 + q_1 x + \dots + q_M x^M} ,$$

subject to the requirement

$$[M,N]_{F(z,x)} - F(z,x) = O\left[x^{M+N+1}\right] .$$

The PPA $[M,N]_{f(z)}$ is defined as the standard PA $[M,N]_{F(z,x)}$ calculated at x = 1. Setting N = n+m and M = n we can write, when $m \geq -1$ and $n \geq 0$, in compact form

$$[n,n+m]_F = H_{n+1}^{(m)}\{f_r\} \,/\, H_n^{(m)}\{\Delta^2 f_r\} , \tag{2.2}$$

where $\Delta^0 f_r = f_r$, $\Delta^p f_r = \Delta^{p-1} f_{r+1} - \Delta^{p-1} f_r$ for p > 0 and the $H_k^{(s)}$ are the Hankel determinants defined by

$$H_k^{(s)}\{f_r\} = \begin{vmatrix} f_s & f_{s+1} & \dots & f_{s+k-1} \\ f_{s+1} & f_{s+2} & \dots & f_{s+k} \\ \vdots & \vdots & & \vdots \\ f_{s+k-1} & f_{s+k} & \dots & f_{s+2k-2} \end{vmatrix}$$

for k > 0, $H_0^{(s)}\{f_r\} \equiv 1$, $f_r = \sum_{n=0}^{r} c_n x^n$, for $r \geq 0$ and $f_{-1} = 0$.

III. GENERATING FUNCTION FOR LEGENDRE POLYNOMIALS

The expansion involved is (with $a_n = u^n$)

$$K(z,u) = \sum_{n=0}^{\infty} u^n P_n(z) = (u^2 - 2uz + 1)^{-1/2} . \tag{3.1}$$

Assuming that $|u| < r^{-1}$ $(r > 1)$, the elliptical domain of convergence of (3.1)is E_r given by

$$E_r = \{ z \,/\, z = \tfrac{1}{2}(t + t^{-1}) ,\ r^{-1} < |t| < r \} .$$

Let us consider z fixed and out of the interval [-1,1] and regard (3.1)as a power series in u . It is easy to see from Eqs.(2.1) and (2.2), that the PPA [n,n+m] to our given Legendre series is exactly equal to the ordinary PA [n,n+m] to this power series.

Let us now recall an integral representation for Legendre polynomials, valid for z out of [-1,1] [11]

$$P_n(z) = \frac{1}{\pi}\int_0^{\pi}\left[z + (z^2-1)^{\frac{1}{2}}\cos t\right]^n dt ,$$

which after choosing a branch of $(z^2-1)^{1/2}$ and making an appropriate change of variables can be expressed as

$$P_n(z) = \frac{1}{\pi}\int_{a_-}^{a_+}\frac{x^n dx}{(2xz-1-x^2)^{\frac{1}{2}}} , \tag{3.2}$$

where $a_\pm = z \pm (z^2-1)^{1/2}$. Now, by replacing (3.2) into (3.1) we may interchange the order of integration and summation for $|u| < r^{-1}$ ($r > 1$) and $z \in E_r$, to obtain

$$\sum_{n=0}^{\infty} u^n P_n(z) = \frac{1}{\pi}\int_{a_-}^{a_+}\frac{dx}{1-xz}\ \frac{1}{(2xz-1-x^2)^{1/2}} . \tag{3.3}$$

The hypothesis of Nuttall's theorem (see appendix), can now be readily seen to hold. As a consequence, it follows that the sequence of PA's [n,n-1] to the power series in u tends to K(z;u) when $n \to \infty$ uniformly on every compact region of the u-plane cut along the curve $u = 1/v$ with

$$v = (z^2-1)^{\frac{1}{2}} t + z , \quad (-1 \leq t \leq 1) . \tag{3.4}$$

Assuming now that u is fixed, (3.4) also gives the curve on the z-plane (out of the segment [-1,1]) where the sequence of PPA's [n,n-1] to the Legendre series chooses to simulate the cut through its distribution of poles and zeroes. If we restrict ourselves to real u such that $0 < u < 1$, to simplify the discussion, it is then easy to see that the curve involved is the segment $[\frac{1}{2}(u + u^{-1}), \infty]$ which coincides with the cut of the function. Our arguments can be repeated for $-1 < z < 1$, by only replacing everywhere $(z^2-1)^{1/2}$ by $i(1-z^2)^{1/2}$, in order to prove the convergence of the same sequence of PPA's. Furthermore, for $z = \pm 1$ our Legendre series reduces to a geometrical series defining $(1 \pm u)^{-1}$. In this case, the first member of the sequence, the [1,0] PPA, gives the exact result.

A numerical study has been performed in order to test the practical significance of our results. We have taken u = 0.5. With this choice, the domain of convergence of the series is the interior of an ellipse with the semi-major axis equal to $[(u + u^{-1})/2]_{u=0.5} = 1.25$, and foci at ± 1 (note that R = 2 in this case). We display some representative results in Tables I and II, for the sequence [n,n-1], using up to the first 13 terms of the series *). The sequence was recurrently generated for each z by using the Eta algorithm [12]. In Table I, comparison is made with the partial sum $\sum_{n=0}^{12} u^n P_n(z)$, on the real axis. The results in Table II correspond to points on an elliptical curve given parametrically by $z = (2\cos\theta , 6\sin\theta/5)$ for $0 \leq \theta \leq \pi$, having the same excentricity as that above, but cutting the real axis at x = 2. The comparison with the partial sums is here meaningless since we are out of their region of convergence.

Let us comment on the general features. In both cases the accuracy is seen to increase quite rapidly with the order of the approximant, for a given z. Considering Table I, in particular, we note its great improvement close to $z = \pm 1$, as can be expected following our discussion above. Moreover, f_{12} breaks down close to $z = \pm 1.25$, limits of its convergence domain, while the PPA's still converge <u>out</u> of that region, as also verified in Table II. In the latter case, we also note a certain oscillatory behaviour for the relative error values, which indicate the presence of regular dips, as θ varies. Finally, we note that the accuracy of the approximants tends to decrease as we approach the branch point at z = 1.25. More generally, this happens as we approach the segment $[1.25,\infty]$ where the approximants simulate the cut of f(z) by placing their poles and zeroes.

IV. THE SCATTERING AMPLITUDE FOR THE COULOMB POTENTIAL

The amplitude is well known exactly for $z \neq 1$ and is given in terms of the parameter γ by

$$f(z) = \frac{-\gamma^2}{1-z}\exp\left\{2i\sigma_0 - i\gamma\log\left[(1-z)/2\right]\right\} ,$$

where $\sigma_k = \arg\Gamma(k + 1 + i\gamma)$. It has a <u>formal</u> expansion as series in Legendre polynomials

*) The [n,n-1] requires the first 2n terms of the series for its calculation.

$$f(z) \doteq \frac{|\gamma|}{2i} \sum_{k=0}^{\infty} (2k+1) \exp [2i\sigma_k] P_k(z) ,$$

divergent for all z. *) In this case the convergence has only been proved for the row sequences of PPA's and for $-1 \leq z < 1$, i.e., for the physical values of z for which f(z) is finite [4].

We have also made a numerical study for this example, setting $\gamma = 1$. The same type of general features discussed previously, regarding the convergence of the sequence of [n,n-1] PPA's, were seen to be present for this case, when appropriate. In particular, the sequence breaks down when approaching the cut $[1,\infty]$. Table III shows some representative results on the real axis.

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*) This series can be shown to be convergent in the distributional sense to a "smeared" version of f(z) in [-1,1] [13].

APPENDIX

Nuttall's theorem *)

Consider the function f(z) defined by

$$f(z) = \int_a^b \frac{\phi(v)\, dv}{1 - vz} , \qquad (A.1)$$

with a,b and $\phi(v)$ possibly complex and such that by defining

$$h(\theta) = \phi\left\{\tfrac{1}{2}\left[(b-a)\cos\theta + a + b\right]\right\} |\sin\theta| , \qquad (A.2)$$

the following statements hold, for $-\pi \leq \theta \leq \pi$,

i) A and B independent of θ exist such that

$$A > |h(\theta)| > B > 0 ,$$

ii) positive L and λ exist, independent of θ, such that

$$\left| \frac{h(\theta+\delta) - h(\theta)}{h(\theta+\delta)\, h(\theta)} \right| < B^{-2} L\, |\log \delta|^{-1-\lambda}$$

Then, the PA [n,n-1] to f(z), based on its expansion in powers of z, converges uniformly to f(z) when $n \to \infty$, in any closed bounded region of the z-plane cut along the arc $z = 1/v$, with

$$v = \tfrac{1}{2}\left[(b-a)t + a + b\right]$$

and $-1 \leq t \leq 1$.

Comparing Eqs.(A.1) and (3.3), we may identify $a = a_-$, $b = a_+$ and $\phi(v) = (2vz - 1 - v^2)^{-1/2}$ and by direct substitution in (A.2) verify that $h(\theta) = (z^2 - 1)^{-1/2} \neq 0$ and independent of θ, and hence the hypotheses of the theorem are seen to hold for that case.

*) We give it here as it appears in Ref.14; it is, however, included in a more general theorem by Nuttall and Singh [15].

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Table I

$\log_{10}[||f_A|^2 - |f|^2|/|f|^2]$ as function of z, for z on the real axis. f_A is, alternatively, an approximant [n,n-1] or f_{12} .

z	[3,2]	[4,3]	[5,4]	[6,5]	$\sum_{n=0}^{12} u_n P_n(z)$
1.14	-2.07	-2.95	-3.84	-4.73	-1.11
1.04	-4.30	-5.94	-7.57	< -9.00	-2.53
0.94	-4.22	-5.83	-7.44	< -9.00	-4.35
0.54	-2.83	-3.98	-5.12	-6.27	-4.34
0.04	-3.11	-4.35	-5.59	-6.83	-5.35
-0.46	-3.94	-5.45	-6.97	-8.48	-4.56
-0.96	-7.35	< -9.00	< -9.00	< -9.00	-4.01
-1.06	-6.83	< -9.00	< -9.00	< -9.00	-2.36
-1.16	-5.56	-7.62	< -9.00	< -9.00	-1.25
-1.26	-4.94	-6.79	-8.63	< -9.00	-0.43
-2.16	-3.08	-4.30	-5.53	-6.75	> 0
-3.76	-2.11	-3.01	-3.91	-4.81	> 0

Table II

Caption as in Table I for $z = (2\cos\theta, 6\sin\theta/5)$ $(0 < \theta < \pi)$

$\theta \times 50/\pi$	[3,2]	[4,3]	[5,4]	[6,5]
4	> 0	-0.20	-0.11	-0.42
7	-0.11	-0.60	-0.77	-1.10
13	-1.12	-1.74	-2.35	-3.00
15	-1.49	-2.29	-3.21	-4.95
16	-1.70	-2.69	-4.99	-4.05
17	-1.96	-3.52	-3.57	-3.99
19	-3.06	-2.99	-3.52	-4.24
23	-2.38	-3.15	-4.22	-6.14
24	-2.50	-3.69	-5.22	-5.62
25	-2.70	-4.64	-4.93	-6.03
30	-3.01	-4.28	-5.17	-7.65
32	-3.72	-4.22	-5.90	-6.64
33	-4.03	-4.30	-6.26	-6.75
35	-3.35	-4.70	-5.73	-8.03
36	-3.28	-5.32	-5.78	-7.32
39	-3.33	-4.63	-6.55	-7.38
40	-3.43	-4.60	-6.08	-8.29
43	-5.83	-4.89	-5.95	-7.18
44	-3.90	-5.29	-6.10	-7.22
45	-3.61	-5.48	-6.49	-7.40
46	-3.45	-4.94	-6.70	-7.98
47	-3.[illegible]	-4.73	-6.15	-7.66
50	-3.25	-4.54	-5.82	-7.11

Table III

Caption as in Table I, for the Coulombian scattering amplitude.

z	[3,2]	[4,3]	[5,4]	[6,5]
0.90	-0.01	-0.01	-1.98	-0.31
0.30	-0.26	-0.52	-0.96	-1.68
-0.20	-0.82	-2.59	-2.23	-3.47
-0.80	-1.39	-2.41	-3.82	-4.91
-1.00	-1.99	-3.45	-4.95	-6.47
-1.20	-1.43	-2.58	-3.67	-4.85
-1.70	-0.98	-1.83	-2.74	-3.71
-2.20	-0.74	-1.47	-2.23	-3.01
-2.80	-0.57	-1.21	-1.88	-2.54
-3.40	-0.48	-1.03	-1.66	-2.28
-4.00	-0.42	-0.91	-1.49	-2.10

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IC/81/89 Trieste International Symposium on Core Level Excitations in Atoms, Molecules and Solids, 22-26 June 1981 (Extended abstracts).

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