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DIAGONAL CONVERGENCE OF THE REMAINDER PADÉ APPROXIMANTS FOR THE HURWITZ ZETA FUNCTION

M. PRÉVOST AND T. RIVOAL

ABSTRACT. The Hurwitz zeta function $\zeta(s, a)$ admits a well-known (divergent) asymptotic expansion in powers of $1/a$ involving the Bernoulli numbers. Using Wilson orthogonal polynomials, we determine an effective bound for the error made when this asymptotic series is replaced by nearly diagonal Padé approximants. By specialization, we obtain new fast converging sequences of rational approximations to the values of the Riemann zeta function at every integers ≥ 2 . The latter can be viewed, in a certain sense, as analogues of Apéry's celebrated sequences of rational approximations to $\zeta(2)$ and $\zeta(3)$.

1. INTRODUCTION

Hurwitz zeta function is defined, for $\Re(a) > 0$ and $\Re(s) > 1$, as

$$\zeta(s, a) = \sum_{k=0}^{\infty} \frac{1}{(k+a)^s}.$$

It is assumed that $a \mapsto \log(a+k)$ is defined with its principal determination. For fixed a such that $\Re(a) > 0$, $\zeta(s, a)$ can be analytically continued to $s \in \mathbb{C} \setminus \{1\}$, with a pole at $s = 1$.

The goal of this paper is to construct rapidly convergent sequences of complex numbers to $\zeta(s, a)$, which are in fact sequences of rational numbers when $s \geq 2$ and $a \geq 1$ are integers. Our method is based on the construction of *remainder Padé approximants* to (analytic continuation of) $\zeta(s, a)$, ie to ordinary Padé approximants to the remainder series $\sum_{k=n+1}^{\infty} \frac{1}{(k+a)^s}$ when n is viewed as a variable. We refer to [5, 6, 7, 8, 9] for other examples of this method. In the present situation, we first remark that, for any integer $n \geq 0$, we have the trivial relation

$$\zeta(s, a) = \sum_{k=0}^{n-1} \frac{1}{(k+a)^s} + \zeta(s, n+a). \quad (1.1)$$

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It is known that $t^{1-s}\zeta(s, 1/t)$ (defined with the principal determination of $\log(t)$) admits an asymptotic expansion in Poincaré sense:

$$t^{1-s}\zeta(s, 1/t) \sim \frac{1}{s-1} + \frac{t}{2} + \sum_{k=1}^{\infty} \frac{(s)_{2k-1}}{(2k)!} B_{2k} t^{2k}, \quad t \rightarrow 0, \Re(t) > 0 \quad (1.2)$$

where $(B_{2k})_{k \geq 1}$ is the sequence of Bernoulli numbers of positive even indices. With $t = 1/(n+a)$, we deduce from (1.2) an asymptotic expansion in powers of $1/(n+a)$ of $\zeta(s, n+a)$ on the right-hand side of (1.1), which we want to “replace” by certain of its Padé approximants evaluated at $1/(n+a)$. We provide a derivation of (1.2) for the reader’s convenience in §2.

For any $s > 0$, let us consider the formal power series

$$\Phi_s(z) := \sum_{n=0}^{\infty} \frac{(s)_{2n+1}}{(2n+2)!} B_{2n+2} (-z)^n, \quad (1.3)$$

which appears on the right hand side of (1.2). It is a divergent series for all $z \neq 0$. As we shall see, it is also the asymptotic expansion at $z = 0, z \notin [0, +\infty)$ of a function analytic in $\mathbb{C} \setminus [0, \infty)$:

$$\widehat{\Phi}_s(z) = \int_0^{+\infty} \frac{\mu_s(x)}{1-zx} dx,$$

where $\mu_s(x)$ is an explicit weight function given in §2. The assumption that s is real ensures the positivity of $\mu_s(x)$, which is crucial for us.

We shall prove in §5 an estimate (Proposition 2) for the error term

$$\varepsilon_{k,s}(z) := \widehat{\Phi}_s(z) - [k/k]_{\Phi_s}(z).$$

Using Carleman’s criterion [4, p. 84], the first author proved in [7] the convergence of $\varepsilon_{k,s}(z)$ to 0 as $k \rightarrow +\infty$, for fixed s and z . The bound (5.1) given in Proposition 2 is useless when z is fixed but it becomes interesting for certain choices of $z = z(k) \rightarrow 0$ as $k \rightarrow +\infty$. This is the situation we are in, and this enables us to construct sequences that converge quickly to $\zeta(a, s)$. If $s, a \in \mathbb{N}$, these are sequences of rational numbers.

Theorem 1. *Let $s > 0, s \neq 1$ and $a \in \mathbb{C}$ be such that $\Re(a) > 0$. Set $a_n := n + a$. Then, for every large enough integer n and any integer $k \geq 0$, we have*

$$\zeta(s, a) = \sum_{k=0}^{n-1} \frac{1}{(k+a)^s} + \frac{1}{(s-1)a_n^{s-1}} + \frac{1}{2a_n^s} + \frac{1}{a_n^{s+1}} [k/k]_{\Phi_s} \left(-\frac{1}{a_n^2} \right) + \varepsilon_{k,s} \left(-\frac{1}{a_n^2} \right), \quad (1.4)$$

where

$$|\varepsilon_{k,s}(-1/a_n^2)| \leq D_s \frac{(2k+2\rho)\Gamma(2k+\rho+1)^2}{|a_n|^{4k+2} (4k+2\rho+1)(2k+1) \binom{4k+2\rho}{2k+1}^2}, \quad (1.5)$$

where $\rho := \frac{1}{2}(m+7)$ and $D_s := (2\pi)^s m!/\Gamma(s)$ and $m := \lfloor s \rfloor$.

The right-hand side of (1.5) tends to 0 as $n \rightarrow +\infty$ slowly if k is fixed and much more rapidly if k is chosen as a function of n of (sub)linear growth. “Large enough integer n ” means that n must be such that $\Re(1/(n+a)^2) > 0$; in particular we can take $n \geq 0$ if $a > 0$. The term $\frac{1}{s-1}$ in (1.2) reflects the fact that $s = 1$ is a pole of $\zeta(s, a)$ (see (2.1) below). However, the formal series $\Phi_s(z)$ is well-defined for $s = 1$ and its Padé approximants can be computed as well. We did that in [8] and proved a result similar to Theorem 1 for the Digamma function defined by

$$\Psi(a) := -\gamma + \sum_{k=0}^{\infty} \left(\frac{1}{k+1} - \frac{1}{k+a} \right),$$

which can be viewed as a convergent version of $-\zeta(1, a)$. The results of the present paper therefore complement those of [8]. Of particular importance in Theorem 1 is the case when $a = 1$ because our results enable to construct fast convergent sequences of real numbers to the values of the Riemann zeta function $\zeta(s)$.

Corollary 1. *Let $r \in \mathbb{Q}$ such that $0 < r < 2e$. Let $s > 0$, $s \neq 1$. Then, for every integer $n \geq 1$ such that rn is an integer, we have*

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{(s-1)n^{s-1}} - \frac{1}{2n^s} + \frac{1}{n^{s+1}} [rn/rn]_{\Phi_s} \left(-\frac{1}{n^2} \right) + \delta_{r,s,n}, \quad (1.6)$$

where

$$\limsup_{n \rightarrow +\infty} |\delta_{r,s,n}|^{1/n} \leq \left(\frac{r}{2e} \right)^{4r}. \quad (1.7)$$

The paper is organized as follows. In §2, we present a Stieljes type integral representation of $\zeta(s, a)$ that enables to analytically continue it, and we deduce some properties of $\widehat{\Phi}_s(z)$. In §3, we obtain a bound for the weight function $\mu_s(x)$. This bound displays a connection with Wilson’s polynomials for the weight function $|\Gamma(\alpha + ix)\Gamma(\beta + ix)|^2$. We use this connection in §5 to prove an intermediate result (Proposition 2), from which Theorem 1 is then easily deduced in §6. In §7, we extend the previous results to the case s is negative. We conclude in §8 with some remarks on the special case $s \in \mathbb{N}$ in Corollary 1.

2. CONSEQUENCES OF AN INTEGRAL REPRESENTATION OF $\zeta(s, a)$

The first author proved in [7] that for every $s, a \in \mathbb{C}$ such that $\Re(s) > 0$, $s \neq 1$, $\Re(a) > 0$, and every non-negative integer $m > \Re(s) - 1$, we have

$$\zeta(s, a) = \frac{1}{a^{s-1}} \left(\frac{1}{s-1} + \frac{1}{2a} + \int_0^{+\infty} \frac{\omega_s(x)}{a^2 + x^2} dx \right) \quad (2.1)$$

where $\log(a)$ is defined with its principal determination and the weight function ω_s is defined (for any $s \in \mathbb{C}$ and $x \geq 0$) by

$$\omega_s(x) := \frac{2(-1)^m x^s}{\Gamma(s)\Gamma(m+1-s)} \int_x^{+\infty} (t-x)^{m-s} \frac{d^m}{dt^m} \left(\frac{1}{e^{2\pi t} - 1} \right) dt. \quad (2.2)$$

The function $t \mapsto (t-x)^{m-s}$ and $x \mapsto x^s$ are defined with the principal determinations of $\log(t-x)$ and $\log(x)$. Note that $\omega_s(x)$ is really independent of the integer m , as an integration by parts shows. When $s \geq 1$ is an integer, we take $m = s$ so that

$$\omega_s(x) = \frac{2(-1)^{s-1}x^s}{(s-1)!} \frac{d^{s-1}}{dx^{s-1}} \left(\frac{1}{e^{2\pi x} - 1} \right) \in L^1(\mathbb{R}).$$

In that case, (2.1) was known earlier, see [4, p. 230] for instance. When s is not an integer, we observe that $|\omega_s(x)| \gg x^{\Re(s)}$ in a neighborhood of $x = 0$, while $|\omega_s(x)| \ll e^{-2\pi x}$ as $x \rightarrow +\infty$. Hence, $\omega_s(x) \in L^1(\mathbb{R})$ when $\Re(s) > 0$.

For $\Re(s) > 0$ and $x \geq 0$, we define $\mu_s(x) := \frac{\omega_s(\sqrt{x})}{2\sqrt{x}} \in L^1(\mathbb{R}^+)$ and set

$$\widehat{\Phi}_s(z) := \int_0^{+\infty} \frac{\mu_s(x)}{1-zx} dx.$$

This defines a function of z analytic in $\mathbb{C} \setminus [0, +\infty)$. Provided $\Re(s) > 0, s \neq 1$, Eq. (1.2) can then be rewritten as

$$t^{1-s} \zeta(s, 1/t) = \frac{1}{s-1} + \frac{t}{2} + t^2 \widehat{\Phi}_s(-t^2) \quad (2.3)$$

for any t such that $\Re(1/t) > 0$.

Now, for any integer $k \geq 0$, we have

$$(-1)^k \frac{B_{2k+2}}{2k+2} = \int_0^{+\infty} x^{2k} \omega_1(x) dx = \int_0^{+\infty} x^k \mu_1(x) dx. \quad (2.4)$$

This classical identity is reproved in [8, Proposition 1] for instance. It is proved in [7, Theorem 2] that, more generally, for every integer $k \geq 0$ and every s such that $\Re(s) > 0$, we have

$$\frac{(s)_{2k+1}}{(2k+2)!} (-1)^k B_{2k+2} = \int_0^{+\infty} x^{2k} \omega_s(x) dx = \int_0^{+\infty} x^k \mu_s(x) dx. \quad (2.5)$$

It follows from (2.5) that, for any integer $N \geq 0$, $z \in \mathbb{C} \setminus [0, +\infty)$ and $\Re(s) > 0$,

$$\widehat{\Phi}_s(z) = \sum_{k=0}^{N-1} \frac{(s)_{2k+1}}{(2k+2)!} B_{2k+2} (-z)^k + z^N \int_0^{+\infty} \frac{x^N}{1-zx} \mu_s(x) dx$$

and this justifies the claim that the divergent series $\Phi_s(z)$ is the asymptotic expansion at $z = 0, z \notin [0, +\infty)$ of $\widehat{\Phi}_s(z)$. Moreover, using (2.3), this also justifies the asymptotic expansion (1.2) in the Introduction.

3. BOUNDS FOR THE WEIGHT $\omega_s(x)$

The goal of this section is to prove the following

Proposition 1. *For any $s > 0$ and any $x \geq 0$, we have*

$$0 \leq \Gamma(s)x\omega_s(x) \leq 2(2\pi)^{s-1}m! G\left(\frac{m+5}{2}, 1, x\right),$$

where $m := \lfloor s \rfloor$ and

$$G(\alpha, \beta, x) := |\Gamma(\alpha + ix)\Gamma(\beta + ix)|^2. \quad (3.1)$$

3.1. Intermediate bounds. We set $G(\alpha, \beta, x) := |\Gamma(\alpha + ix)\Gamma(\beta + ix)|^2$ for $\alpha, \beta > 0$ and $x \in \mathbb{R}$. We prove here the

Lemma 1. (i) For every $x > 0$ and every integer $m \geq 0$, we have

$$0 \leq (-1)^m \frac{d^m}{dx^m} \left(\frac{1}{e^{2\pi x} - 1} \right) \leq (2\pi)^m m! \frac{e^{2\pi m x}}{(e^{2\pi x} - 1)^{m+1}}. \quad (3.2)$$

(ii) For every $x \geq 0$ and every integer $m \geq 0$, we have

$$\left(\frac{x}{1 - e^{-2\pi x}} \right)^{m+1} G(2, 1, x) \leq G\left(\frac{m+5}{2}, 1, x\right). \quad (3.3)$$

Proof. The proof is tedious but without any difficulties. We will implicitly use some classical properties of the Gamma function.

(i) For $x > 0$, set $\nu(x) = \frac{1}{e^x - 1}$. We have

$$\frac{d^m \nu(x)}{dx^m} = (-1)^m \nu(x)^{m+1} \sum_{k=1}^m a_k^{(m)} e^{kx},$$

where the $a_k^{(m)}$ satisfy the linear recursion

$$a_k^{(m+1)} = (m+2-k)a_{k-1}^{(m)} + ka_k^{(m)}, \quad k = 1, \dots, m+1$$

with the convention that $a_1^{(0)} = a_1^{(1)} = 1$, $a_0^{(m)} = 0$, $a_{m+1}^{(m)} = 0$ for any $m \geq 1$. Since $a_1^{(1)} = 1$, we obtain by induction that for all $k = 1, \dots, m$, $a_k^{(m)} \geq 0$, $a_{m+1}^{(m+1)} = a_m^{(m)} = 1$ and

$$\sum_{k=1}^{m+1} a_k^{(m+1)} = (m+1) \sum_{k=1}^m a_k^{(m)} = (m+1)!.$$

It follows that

$$(-1)^m \frac{d^m \nu(x)}{dx^m} = \nu(x)^{m+1} \sum_{k=1}^m a_k^{(m)} e^{kx}.$$

Hence,

$$0 \leq (-1)^m \frac{d^m \nu(x)}{dx^m} \leq \nu(x)^{m+1} e^{mx} \sum_{k=1}^m a_k^{(m)} = m! \frac{e^{mx}}{(e^x - 1)^{m+1}}.$$

In other words, we have

$$0 \leq (-1)^m \frac{d^m}{dx^m} \left(\frac{1}{e^{2\pi x} - 1} \right) \leq (2\pi)^m m! \frac{e^{2\pi m x}}{(e^{2\pi x} - 1)^{m+1}}$$

as expected.

(ii) It will be enough to prove that, for every integer $p \geq 1$ and every $x \geq 0$, we have

$$\frac{G(p, 1, x)}{G(p + \frac{1}{2}, 1, x)} \frac{x}{1 - e^{-2\pi x}} \leq 1 \quad \text{and} \quad \frac{G(p + \frac{1}{2}, 1, x)}{G(p + 1, 1, x)} \frac{x}{1 - e^{-2\pi x}} \leq 1.$$

Eq. (3.3) will then follow from this two bounds by induction on $m \geq 0$.

Firstly, we have

$$\begin{aligned}
\frac{G(p, 1, x)}{G(p + \frac{1}{2}, 1, x)} \frac{x}{1 - e^{-2\pi x}} &= \frac{x}{1 - e^{-2\pi x}} \frac{|\Gamma(p + ix)|^2}{|\Gamma(p + \frac{1}{2} + ix)|^2} \\
&= \frac{x}{1 - e^{-2\pi x}} \frac{|p - 1 + ix|^2 |p - 2 + ix|^2 \cdots |ix|^2 |\Gamma(ix)|^2}{|p - \frac{1}{2} + ix|^2 |p - \frac{3}{2} + ix|^2 \cdots |\frac{1}{2} + ix|^2 |\Gamma(\frac{1}{2} + ix)|^2} \\
&= \frac{x}{1 - e^{-2\pi x}} \frac{|p - 1 + ix|^2 |p - 2 + ix|^2 \cdots |ix|^2 \frac{\pi}{x \sinh(\pi x)}}{|p - \frac{1}{2} + ix|^2 |p - \frac{3}{2} + ix|^2 \cdots |\frac{1}{2} + ix|^2 \frac{\pi}{\cosh(\pi x)}} \\
&\leq \frac{x^2}{\frac{1}{4} + x^2} \coth(\pi x) \frac{1}{1 - e^{-2\pi x}} = \frac{x^2}{\frac{1}{4} + x^2} \frac{1 + e^{-2\pi x}}{(1 - e^{-2\pi x})^2} \leq 1.
\end{aligned}$$

The last inequality is proved as follows: for all $x \geq 0$, we have

$$\begin{aligned}
1 - \frac{x^2}{\frac{1}{4} + x^2} \frac{1 + e^{-2\pi x}}{(1 - e^{-2\pi x})^2} &= \frac{e^{4\pi x} - 2(1 + 6x^2)e^{2\pi x} + 1 + 4x^2}{(1 - e^{2\pi x})^2(1 + 4x^2)} \\
&\geq \frac{e^{4\pi x} - 2(1 + 6x^2)e^{2\pi x} + 1 - 4x^2 - 48x^3}{(1 - e^{2\pi x})^2(1 + 4x^2)} \\
&= \frac{(e^{2\pi x} - 1 + 4x)(e^{2\pi x} - 1 - 4x - 12x^2)}{(1 - e^{2\pi x})^2(1 + 4x^2)} \geq 0,
\end{aligned}$$

as the study of the variations of $e^{2\pi x} - 1 + 4x$ and $e^{2\pi x} - 1 - 4x - 12x^2$ shows.

Similarly, we have

$$\begin{aligned}
\frac{G(p + \frac{1}{2}, 1, x)}{G(p + 1, 1, x)} \frac{x}{1 - e^{-2\pi x}} &= \frac{x}{1 - e^{-2\pi x}} \frac{|p - \frac{1}{2} + ix|^2 |p - \frac{3}{2} + ix|^2 \cdots |\frac{1}{2} + ix|^2 \frac{\pi}{\cosh(\pi x)}}{|p + ix|^2 |p - 1 + ix|^2 \cdots |ix|^2 \frac{\pi}{x \sinh(\pi x)}} \\
&\leq \frac{x}{1 - e^{-2\pi x}} \frac{\frac{\pi}{\cosh(\pi x)}}{|ix|^2 \frac{\pi}{x \sinh(\pi x)}} = \frac{\tanh(\pi x)}{1 - e^{-2\pi x}} = \frac{e^{\pi x}}{e^{\pi x} + e^{-\pi x}} \leq 1.
\end{aligned}$$

This completes the proof. \square

3.2. Proof of Proposition 1.

We can now prove Proposition 1. Since for every $x > 0$ and every integer $m \geq 0$, we have

$$(-1)^m \frac{d^m}{dx^m} \left(\frac{1}{e^{2\pi x} - 1} \right) \geq 0$$

(by the lower bound in Lemma 1(i)), the integral definition (2.2) of $\omega_s(x)$ shows that for any $x \geq 0$ and any $s > 0$, we have $x\omega_s(x) \geq 0$ and $\Gamma(s) > 0$.

We now proceed to get the upper bound. From now on, $m := \lfloor s \rfloor$, so that $0 \leq s - m < 1$. Starting from (2.2) and the upper bound in Lemma 1(i), we obtain in succession

$$\begin{aligned} \Gamma(s)\omega_s(x) &\leq \frac{2x^s(2\pi)^m m!}{\Gamma(m+1-s)} \int_x^\infty (t-x)^{m-s} \frac{e^{2\pi mt}}{(e^{2\pi t}-1)^{m+1}} dt \\ &= \frac{2x^s(2\pi)^m m!}{\Gamma(m+1-s)} \int_x^\infty (t-x)^{m-s} e^{-2\pi t} \left(\frac{e^{2\pi t}}{e^{2\pi t}-1} \right)^{m+1} dt \\ &\leq \frac{2x^s(2\pi)^m m!}{\Gamma(m+1-s)} \left(\frac{e^{2\pi x}}{e^{2\pi x}-1} \right)^{m+1} \int_x^\infty (t-x)^{m-s} e^{-2\pi t} dt \\ &= 2x^{s-m-1} (2\pi)^{s-1} m! \left(\frac{x}{1-e^{-2\pi x}} \right)^{m+1} e^{-2\pi x} \end{aligned}$$

We now use that, for $x \geq 0$,

$$e^{-2\pi x} \leq \pi^2 \frac{x^2}{\sinh(\pi x)^2} =: G(1, 1, x).$$

Indeed, we have for $x \geq 0$

$$\pi^2 x^2 - \sinh(\pi x)^2 e^{-2\pi x} = \frac{1}{4} (2\pi x - 1 + e^{-2\pi x}) (2\pi x + 1 - e^{-2\pi x}) \geq 0.$$

Hence,

$$\begin{aligned} \Gamma(s)x\omega_s(x) &\leq 2x^{s-m}(2\pi)^{s-1}m! \left(\frac{x}{1-e^{-2\pi x}} \right)^{m+1} G(1, 1, x) \\ &\leq 2(2\pi)^{s-1}m! \left(\frac{x}{1-e^{-2\pi x}} \right)^{m+1} (1+x^2) G(1, 1, x) \quad (\text{since } x^{s-m} \leq 1+x^2) \\ &= 2(2\pi)^{s-1}m! \left(\frac{x}{1-e^{-2\pi x}} \right)^{m+1} G(2, 1, x) \leq 2(2\pi)^{s-1}m! G\left(\frac{m+5}{2}, 1, x\right) \end{aligned}$$

by Lemma 1(ii).

4. WILSON'S POLYNOMIALS

We now make a crucial observation: $G(\alpha, \beta, x)$ is Wilson's weight on $(0, +\infty)$, for which the orthogonal polynomials are explicitly known; see [2, 11]. We review these facts in this section.

Let $\alpha, \beta > 0$. Wilson's polynomials are defined by

$$P_n(\alpha, \beta, x) := i^n {}_3F_2 \left[\begin{matrix} -n, n+2\alpha+2\beta-1, \beta-ix \\ \alpha+\beta, 2\beta \end{matrix} ; 1 \right] \in \mathbb{R}[x]$$

and they have the parity of n . The leading coefficient of $P_n(\alpha, \beta, x)$ is

$$(-1)^n \frac{(n+2\alpha+2\beta-1)_n}{(\alpha+\beta)_n (2\beta)_n}.$$

They satisfy the orthogonality relations

$$\int_{-\infty}^{+\infty} P_n(\alpha, \beta, x) P_m(\alpha, \beta, x) G(\alpha, \beta, x) dx = 0, \quad n \neq m,$$

and

$$\int_{-\infty}^{+\infty} P_n^2(\alpha, \beta, x) G(\alpha, \beta, x) dx = \frac{(1)_n (2\alpha)_n (\alpha + \beta - \frac{1}{2})_n}{(2\beta)_n (2\alpha + 2\beta - 1)_n (\alpha + \beta + \frac{1}{2})_n} A(\alpha, \beta),$$

where

$$A(\alpha, \beta) := \int_{-\infty}^{+\infty} G(\alpha, \beta, x) dx = \frac{\Gamma(\alpha) \Gamma(\alpha + \frac{1}{2}) \Gamma(\beta) \Gamma(\beta + \frac{1}{2}) \Gamma(\alpha + \beta) \Gamma(\frac{1}{2})}{\Gamma(\alpha + \beta + \frac{1}{2})}.$$

Consider now the weight function $\gamma(\alpha, \beta, x) := \frac{1}{\sqrt{x}} G(\alpha, \beta, \sqrt{x}) \in L^1(\mathbb{R}^+)$. The sequence of monic orthogonal polynomials $(T_k(\alpha, \beta, x))_k$ on $[0, \infty)$ with respect to $\gamma(\alpha, \beta, x)$ is given by

$$T_k(\alpha, \beta, x) = \frac{(\alpha + \beta)_{2k} (2\beta)_{2k}}{(2k + 2\alpha + 2\beta - 1)_{2k}} P_{2k}(\alpha, \beta, \sqrt{x}).$$

In particular, for all $k \geq 0$,

$$\int_0^{+\infty} T_k^2(\alpha, \beta, x) \gamma(\alpha, \beta, x) dx = \frac{\pi^2 (4k + 2\alpha + 2\beta - 1) (2k)! \Gamma(2k + 2\alpha) \Gamma(2k + 2\beta) \Gamma(2k + 2\alpha + 2\beta - 1)}{2^{8k+4\alpha+4\beta-3} \Gamma(2k + \alpha + \beta + \frac{1}{2})^2}. \quad (4.1)$$

If $\beta = 1$, then

$$T_n(\alpha, 1, x) = \frac{(-1)^n (2n)! (\alpha)_{2n+1}}{(2n + 2\alpha)_{2n+1}} \sum_{j=0}^{2n} \binom{2n+1}{j+1} \binom{2n+2\alpha+j}{j+1} \binom{i\sqrt{x}-1}{j} / \binom{\alpha+j}{j+1}$$

and, after simplification of (4.1),

$$\int_0^{+\infty} T_k^2(\alpha, 1, x) \gamma(\alpha, 1, x) dx = \frac{2\pi(2k+2\alpha)}{(2k+1)(4k+2\alpha+1)} \frac{\Gamma(2k+\alpha+1)^2}{\binom{4k+2\alpha}{2k+1}^2}.$$

5. A BOUND FOR THE PADÉ APPROXIMANTS OF Φ_s

We recall that

$$\widehat{\Phi}_s(z) := \int_0^{+\infty} \frac{\mu_s(x)}{1-zx} dx, \quad z \in \mathbb{C} \setminus [0, +\infty).$$

In this section, we shall prove the following bound.

Proposition 2. *Let $z \in \mathbb{C}$ such that $\Re(z) < 0$, and $s > 0$. For any integer $k \geq 0$, set*

$$\varepsilon_{k,s}(z) := \widehat{\Phi}_s(z) - [k/k]_{\Phi_s}(z).$$

Then,

$$|\varepsilon_{k,s}(z)| \leq C_s |z|^{2k+1} \frac{2\pi(2k+2\rho)\Gamma(2k+\rho+1)^2}{(4k+2\rho+1)(2k+1)\binom{4k+2\rho}{2k+1}^2} \quad (5.1)$$

where $\rho := \frac{1}{2}(m+7)$ and $C_s := (2\pi)^{s-1}m!/\Gamma(s)$ and $m := \lfloor s \rfloor$.

Proof. We first prove a crucial inequality, namely Eq (5.3) below. By Proposition 1, we have for any $x \geq 0$

$$\Gamma(s)\sqrt{x}\omega_s(\sqrt{x}) \leq 2(2\pi)^{s-1}m!G\left(\frac{m+5}{2}, 1, \sqrt{x}\right)$$

where $s > 0$ and $m = \lfloor s \rfloor$. Hence, for $x \geq 0$,

$$\begin{aligned} 0 \leq \Gamma(s)x\mu_s(x) &\leq (2\pi)^{s-1}m!G\left(\frac{m+5}{2}, 1, \sqrt{x}\right) \\ &\leq \frac{(2\pi)^{s-1}m!}{\sqrt{x}}G\left(\frac{m+7}{2}, 1, \sqrt{x}\right) \\ &= (2\pi)^{s-1}m!\gamma\left(\frac{m+7}{2}, 1, x\right) \end{aligned} \quad (5.2)$$

where $\gamma(\alpha, \beta, x) := \frac{1}{\sqrt{x}}G(\alpha, \beta, \sqrt{x}) \in L^1(\mathbb{R}^+)$. In (5.2), we used $\sqrt{x}G(\frac{m+5}{2}, 1, x) \leq |\frac{m+5}{2} + ix|^2 G(\frac{m+5}{2}, 1, x) = G(\frac{m+7}{2}, 1, x)$.

Hence, for $x \geq 0$ and $s > 0$, we have

$$0 \leq x\mu_s(x) \leq C_s \gamma\left(\frac{m+7}{2}, 1, x\right) \quad (5.3)$$

where $C_s := (2\pi)^{s-1}m!/\Gamma(s)$.

For the general properties of Padé approximants and orthogonal polynomials, we refer to [3]. Let $q_k(x) \in \mathbb{R}[x]$ denote the k -th monic orthogonal polynomial with respect to $x\mu_s(x)$ on $[0, +\infty)$. Since $x\mu_s(x) \geq 0$ on $[0, +\infty)$, the roots of $q_k(x)$ are in $[0, +\infty)$ and thus in particular $|q_k(x)| \geq |x|^k$ for all $x \in \mathbb{C}$ such that $\Re(x) \leq 0$. The polynomial $z^k q_k(1/z)$ is the denominator of $[k/k]_{\Phi_s}$ and we have

$$\widehat{\Phi}_s(z) - [k/k]_{\Phi_s}(z) = \frac{z}{q_k(1/z)^2} \int_0^{+\infty} \frac{q_k(x)^2}{1-zx} x\mu_s(x) dx$$

for all $z \in \mathbb{C} \setminus [0, +\infty)$; see the generalization mentioned right after [8, Proposition 3] (where it must be understood that $q_n(u)$ is orthogonal for the weight $u^{m-n+1}\omega(u)$ and not just $\omega(u)$).

Set $\rho = \frac{m+7}{2}$. Eq. (5.3) enables us to apply [8, Proposition 4]: for any $k \geq 0$ and $s > 0$, we have

$$0 \leq \int_0^{+\infty} q_k(x)^2 x\mu_s(x) dx \leq \int_0^{+\infty} T_k(\rho, 1, x)^2 \gamma(\rho, 1, x) dx.$$

It follows that for all $k \geq 0$, $s > 0$ and $z \in \mathbb{C}$ such that $\Re(z) < 0$, we have

$$\begin{aligned} \left| \frac{z}{q_k(1/z)^2} \int_0^{+\infty} \frac{q_k(x)^2}{1-zx} x \mu_s(x) dx \right| &\leq C_s |z|^{2k+1} \int_0^{+\infty} T_k^2(\rho, 1, x) \gamma(\rho, 1, x) dx \\ &\leq C_s |z|^{2k+1} \frac{2\pi(2k+2\rho)}{(2k+1)(4k+2\rho+1)} \frac{\Gamma(2k+\rho+1)^2}{\binom{4k+2\rho}{2k+1}^2}. \end{aligned}$$

Therefore,

$$\left| \widehat{\Phi}_s(z) - [k/k]_{\Phi_s}(z) \right| \leq C_s |z|^{2k+1} \frac{2\pi(2k+2\rho)}{(4k+2\rho+1)(2k+1)} \frac{\Gamma(2k+\rho+1)^2}{\binom{4k+2\rho}{2k+1}^2},$$

which completes the proof of Proposition 2. \square

6. PROOFS OF THEOREM 1 AND COROLLARY 1

Assume that $s > 0$, $s \neq 1$ and $a \in \mathbb{C}$ is such that $\Re(a) > 0$. There exists $N(a) \geq 0$ such that if $n \geq N(a)$, then $\Re(-1/(n+a)^2) < 0$. Hence for $n \geq N(a)$, $\zeta(s, n+a)$ and $\widehat{\Phi}_s(-1/(n+a)^2)$ are both well-defined and we have (with $a_n := n+a$)

$$\begin{aligned} \zeta(s, a) &= \sum_{k=0}^{n-1} \frac{1}{(k+a)^s} + \zeta(s, n+a) \\ &= \sum_{k=0}^{n-1} \frac{1}{(k+a)^s} + \frac{1}{(s-1)a_n^{s-1}} + \frac{1}{2a_n^s} + \frac{1}{a_n^{s+1}} \widehat{\Phi}_s\left(-\frac{1}{a_n^2}\right) \\ &= \sum_{k=0}^{n-1} \frac{1}{(k+a)^s} + \frac{1}{(s-1)a_n^{s-1}} + \frac{1}{2a_n^s} \\ &\quad + \frac{1}{a_n^{s+1}} [k/k]_{\Phi_s}\left(-\frac{1}{a_n^2}\right) + \frac{1}{a_n^{s+1}} \varepsilon_{k,s}\left(-\frac{1}{a_n^2}\right). \end{aligned}$$

This proves (1.4), and (1.5) is a consequence of Proposition 2 with $z = -1/a_n^2$.

To prove Corollary 1, we take $a = 1$ in Theorem 1, change n to $n-1$, take $k = rn$ and set $\delta_{r,s,n} := \varepsilon_{rn,s}(-1/n^2)$. We get (1.6). The lim sup estimate (1.7) comes from Stirling's formula applied to the upper bound for $\varepsilon_{rn,s}(-1/n^2)$ given by Proposition 2.

7. THE CASE s REAL NEGATIVE

In this section, we show that convergence of certain remainder Padé approximants occur in the case where s is negative but only for well chosen degree of the numerators of those approximants. More precisely we don't consider the weight $x\omega_s(x)$ as in Proposition 1 but $x^{s+2p+1}W_s(x)$, with $p \geq 1$, such that $s+2p$ is positive. Thus the convergence will be established for remainder Padé approximants of degree $[n+p, n]$ when n tends to ∞ .

For $\Re(s) < 0$, Eqs. (2.1) and (2.2) become

Theorem 2. Let $s \in \mathbb{C} \setminus \mathbb{Z}_{\leq 0}$ with $\Re(s) < 0$, $a \in \mathbb{C}$ with $\Re(a) > 0$, and an integer $p \geq 1$ such that $\Re(s) + 2p > 0$. Then

$$\zeta(s, a) = a^{-s+1} \left(\frac{1}{s-1} + \frac{1}{2a} + \sum_{k=0}^{p-1} \frac{(s)_{2k+1}}{(2k+2)!} B_{2k+2} a^{-2-2k} + \frac{a^{-2p}(-1)^p}{\Gamma(s)} \int_0^\infty \frac{u^{2p}}{a^2 + u^2} W_s(u) du \right)$$

where the weight function

$$W_s(u) = \frac{2u^s}{\Gamma(1-s)} \int_u^\infty (y-u)^{-s} \frac{dy}{e^{2\pi y} - 1}$$

is non-negative on $[0, +\infty)$.

Proof. We begin with the following formula

$$\begin{aligned} a^s (a^2 + y^2)^{-s/2} \sin(s \arctan(y/a)) \\ = \frac{(-1)^p}{\Gamma(s)\Gamma(1-s)} \int_0^y \frac{a^{1-2p} u^{s+2p} (y-u)^{-s}}{a^2 + u^2} du + \sum_{k=0}^{p-1} \frac{(s)_{2k+1} (y/a)^{2k+1} (-1)^k}{(2k+1)!}, \end{aligned}$$

the proof of which is similar to that in [7].

We recall Hermite's formula for $\zeta(s, a)$, $\Re(a) > 0$, which is a consequence of Plana's summation formula:

$$\zeta(s, a) = \frac{1}{2} a^{-s} + \frac{a^{1-s}}{s-1} + 2 \int_0^\infty (a^2 + y^2)^{-s/2} \sin\left(s \arctan\left(\frac{y}{a}\right)\right) \frac{dy}{e^{2\pi y} - 1}. \quad (7.1)$$

Thus

$$\begin{aligned} \zeta(s, a) &= \frac{1}{2} a^{-s} + \frac{a^{1-s}}{s-1} + \\ &2a^{-s} \int_0^\infty \left(\frac{(-1)^p}{\Gamma(s)\Gamma(1-s)} \int_0^y \frac{a^{1-2p} u^{s+2p} (y-u)^{-s}}{a^2 + u^2} du + \sum_{k=0}^{p-1} \frac{(s)_{2k+1} (y/a)^{2k+1} (-1)^k}{(2k+1)!} \right) \frac{dy}{e^{2\pi y} - 1} \end{aligned}$$

The first term in the integral can be written as

$$\int_0^\infty \int_0^y \frac{u^{s+2p} (y-u)^{-s}}{a^2 + u^2} du \frac{dy}{e^{2\pi y} - 1} = \int_0^\infty \frac{u^{s+2p}}{a^2 + u^2} du \int_u^\infty (y-u)^{-s} \frac{dy}{e^{2\pi y} - 1},$$

where we can apply Fubini's theorem because

$$0 \leq \frac{u^{s+2p} (y-u)^{-s}}{a^2 + u^2} \frac{1}{e^{2\pi y} - 1} \leq 4^{-p} (-s)^{-s} p^{-2p} (2p+s)^{2p+s} \frac{1}{a^2 + u^2} \frac{y^{2p}}{e^{2\pi y} - 1}$$

and the right-hand side is a function of (u, y) integrable on $[0, +\infty) \times [0, +\infty)$. Eq. (2.5) completes the proof. \square

All the previous results for s with $\Re(s) > 0$ are derived from the bound of the weight $\Gamma(s)x\omega_s(x)$ obtained in §3. Thus all the results in the previous sections are true for s negative provided the Padé approximant $[k, k]$ is replaced by $[k+p, k]$. We adapt the same proof as in the previous sections to get the following analogues of Proposition 1, Theorem 1 and Corollary 1 respectively.

Proposition 3. *For $s < 0$, $s \notin \mathbb{Z}_{\leq 0}$, if $p = \lfloor -s/2 \rfloor + 1$ then*

$$0 \leq x^{2p+1}W_s(x) \leq 2(2\pi)^{s-1}G(5/2, 1, x).$$

Theorem 3. *Let $s < 0$, $s \notin \mathbb{Z}_{\leq 0}$ and $a \in \mathbb{C}$ be such that $\Re(a) > 0$. Set $a_n := n + a$. Then, for every large enough integer n and any integer $k \geq 0$, we have*

$$\zeta(s, a) = \sum_{k=0}^{n-1} \frac{1}{(k+a)^s} + \frac{1}{(s-1)a_n^{s-1}} + \frac{1}{2a_n^s} + \frac{1}{a_n^{s+1}}[k+p/k]_{\Phi_s} \left(-\frac{1}{a_n^2} \right) + \varepsilon_{k,s} \left(-\frac{1}{a_n^2} \right), \quad (7.2)$$

where

$$|\varepsilon_{k,s}(-1/a_n^2)| \leq D_s \frac{(2k+2\rho)\Gamma(2k+\rho+1)^2}{|a_n|^{4k+3+2p+s}(4k+2\rho+1)(2k+1)\binom{4k+2\rho}{2k+1}^2}, \quad (7.3)$$

where $\rho := \frac{5}{2}$ and $D_s := (2\pi)^s/\Gamma(s)$ and $p := \lfloor -s/2 \rfloor + 1$.

Corollary 2. *Let $r \in \mathbb{Q}$ such that $0 < r < 2e$. Let $s < 0$, $s \notin \mathbb{Z}_{\leq 0}$ and $p := \lfloor -s/2 \rfloor + 1$. Then, for every integer $n \geq 1$ such that rn is an integer, we have*

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{(s-1)n^{s-1}} - \frac{1}{2n^s} + \frac{1}{n^{s+1}}[rn+p/rn]_{\Phi_s} \left(-\frac{1}{n^2} \right) + \delta_{r,s,n}, \quad (7.4)$$

where

$$\limsup_{n \rightarrow +\infty} |\delta_{r,s,n}|^{1/n} \leq \left(\frac{r}{2e} \right)^{4r}. \quad (7.5)$$

8. THE CASE $a = 1$ AND $s \in \mathbb{N}$

In this section, we discuss the sequences of rational numbers produced by the Padé approximants of $\Phi_s(z)$ when $a = 1$ and $s \geq 1$ is an integer. When $s = 1$, we refer to our paper [8] where we proved in particular that

$$\gamma = \sum_{k=1}^n \frac{1}{k} - \log(n) - \frac{1}{2n} + \frac{1}{n^2}[n-1/n]_{\Phi_1} \left(-\frac{1}{n^2} \right) + \delta_{1,n}, \quad \limsup_{n \rightarrow +\infty} |\delta_{1,n}|^{1/n} \leq (2e)^{-4}.$$

This is very similar to (1.6) when $s \geq 2$ and $r = 1$:

$$\begin{aligned} \zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{(s-1)n^{s-1}} - \frac{1}{2n^s} \\ + \frac{1}{n^{s+1}}[n/n]_{\Phi_s} \left(-\frac{1}{n^2} \right) + \delta_{s,n}, \quad \limsup_{n \rightarrow +\infty} |\delta_{s,n}|^{1/n} \leq (2e)^{-4}. \end{aligned}$$

The change from the Padé approximants $[n - 1/n]$ to $[n/n]$ is not fundamental. It is due to the simplification of a part of our argument, to avoid distinguishing two cases. These equations thus provide sequences of rational numbers $p_{s,n}/q_{s,n}$ (written in reduced form) such that

$$\gamma = \lim_{n \rightarrow +\infty} \left(\frac{p_{1,n}}{q_{1,n}} - \log(n) \right), \quad \zeta(s) = \lim_{n \rightarrow +\infty} \frac{p_{s,n}}{q_{s,n}} \quad (s \geq 2).$$

We computed diagonal Padé approximants $[n/n]_{\Phi_s}$ for various values of the integer $s \geq 1$ for n from 1 to 146. It seems that $|\delta_{s,n}|^{1/n}$ always exists and is not very far from our upper bound $(2e)^{-4}$. The situation is apparently different for the asymptotic behavior of the denominators $q_{s,n}$. On the one hand, if $s = 1$, it seems that $|q_{1,n}|$ grows at least like $c(1)^{n^2 \log(n)(1+o(1))}$ for some constant $c(1) > 1$, while if the integer $s \geq 4$, then it seems that $|q_{s,n}|$ grows at least like $c(s)^{n \log(n)}$ for some constant $c(s) > 1$. On the other hand, if $s \in \{2, 3\}$, $|q_{s,n}|$ seems to grow like $c(s)^{n(1+o(1))}$ for some constant $c(s) > 1$. In fact, if $s \in \{2, 3\}$, then variants of $p_{2,n}/q_{2,n}$ and $p_{3,n}/q_{3,n}$ are known to coincide with the famous sequences Apéry [1] used to prove the irrationality of $\zeta(2)$ and $\zeta(3)$; see [6] or [8, §7] for details.

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