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FAST CONVERGENT SEQUENCES OF APPROXIMATIONS TO STIELTJES' CONSTANTS

M. PRÉVOST AND T. RIVOAL

ABSTRACT. Stieltjes' constants γ_n are the coefficients in the Laurent series for the zeta function $\zeta(s)$ at the pole $s = 1$. We present new sequences of approximations for Stieltjes' constants obtained by generalizing the “remainder Padé approximants” method introduced by the first named author in 1996. Here, we replace Padé approximants (of which poles are connected to zeros of orthogonal polynomials) by Padé type approximants introduced by Brezinski of which poles are chosen *a priori*. The particular case γ_1 is also treated separately using ordinary Padé approximants. The last section of the paper deals with approximations of zeta function in the complex plane.

1. INTRODUCTION

For $a \in \mathbb{C}$, $\Re(a) > 0$, the Hurwitz zeta function is defined as

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

where the Dirichlet series on the right hand side is convergent for $\Re(s) > 1$. It can be analytically continued to $s \in \mathbb{C} \setminus \{1\}$, with a pole at $s = 1$. The generalized Stieltjes constants $\gamma_n(a)$ occur as coefficients in the Laurent series expansion of $\zeta(s, a)$ at the pole $s = 1$:

$$\zeta(s, a) = \frac{1}{s-1} + \sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!} \gamma_\ell(a) (s-1)^\ell.$$

There are numerous representations for them, for instance

$$\gamma_\ell(a) = \lim_{m \rightarrow \infty} \left\{ \sum_{k=0}^m \frac{\ln^\ell(k+a)}{k+a} - \frac{\ln^{\ell+1}(m+a)}{\ell+1} \right\}, \quad \ell = 0, 1, 2, \dots, a \neq 0, -1, -2, \dots$$

If $a = 1$, the generalized Stieltjes constant $\gamma_\ell(a)$ is the usual Stieltjes constant γ_ℓ . More specifically, γ_0 is Euler's constant, usually denoted as γ .

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In [9], using the Digamma function

$$\Psi(z) := \frac{\Gamma'(z)}{\Gamma(z)} = -\gamma + \sum_{n=0}^{\infty} \left(\frac{1}{n+1} - \frac{1}{n+z} \right)$$

for $z \in \mathbb{C} \setminus \mathbb{Z}_{\leq 0}$, the authors constructed approximations of γ as follows. Let $H_n := \sum_{j=1}^n 1/j$ and $\Phi(n) := \gamma - (H_n - \ln(n)) + \frac{1}{2n}$. It is known that

$$\Phi(n) \sim \sum_{k=0}^{\infty} \frac{B_{2k+2}}{2k+2} \frac{1}{n^{2k+2}}, \quad (n \rightarrow +\infty) \quad (1)$$

where the asymptotic expansion is understood in the Poincaré sense.

The remainder Padé approximation method consists in approximating Euler's constant by the sum $(H_n - \ln(n) - \frac{1}{2n}) + [p/q]_{\widehat{\Phi}}$ where $[p/q]$ is a well-chosen Padé approximant of the formal power series

$$\widehat{\Phi}(z) := \sum_{k=0}^{\infty} \frac{B_{2k+2}}{2k+2} (-z)^k.$$

More precisely, the main result of [9] is that for $r \in \mathbb{Q}_{\geq 0}$, $0 < r < 2e$ such that $rn \in \mathbb{N}$, we have

$$\gamma = H_n - \ln(n) - \frac{1}{2n} + \frac{1}{n^2} [rn - 1/rn]_{\widehat{\Phi}}(-1/n^2) + \delta_{r,n}$$

where $\limsup_{n \rightarrow +\infty, rn \in \mathbb{N}} |\delta_{r,n}|^{1/n} \leq (r/2e)^{4r}$. The convergence of the sequence of Padé approximant $[rn - 1/rn]_{\widehat{\Phi}}$ to the function $\widehat{\Phi}$ is a consequence of the following facts: the poles of $[rn - 1/rn]_{\widehat{\Phi}}$ lie on $[0, +\infty)$ and the Padé approximant is computed at $-1/n^2 < 0$.

Being now interested in Stieltjes' constants, we want to use a similar technique. An immediate difficulty arises: the denominators of the Padé approximations for the remainder of γ_ℓ do not necessarily have their roots in $[0, +\infty)$, which prevent us from obtaining any type of convergence. An interesting technic to avoid this difficulty is to make use of Padé type approximants instead of Padé approximants. In this case, it is possible to choose the denominator of the Padé type approximants and thus the poles of the approximant. A possible drawback is that the convergence is *a priori* slower though, as we shall see, it is reasonably fast in our situation.

We shall use the following property of $\gamma_\ell(n)$. For any integer $n \geq 1$, we have

$$\gamma_\ell = \gamma_\ell(n) + \sum_{j=1}^{n-1} \frac{\ln^\ell(j)}{j} \quad (2)$$

which is a consequence of the functional equation $\zeta(s, n) = \zeta(s) - \sum_{j=1}^{n-1} j^{-s}$. The Jensen-Franel integral formula [4] provide a closed form formula for the numbers γ_ℓ :

$$\gamma_\ell(n) = \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell+1} - i \int_0^\infty \frac{dx}{e^{2\pi x} - 1} \left\{ \frac{(\log^\ell(n - ix))}{n - ix} - \frac{(\log^\ell(n + ix))}{n + ix} \right\} \quad (3)$$

for every $\ell, n \in \mathbb{N}$, and where \log is defined with its principal determination as everywhere in this paper. We shall use instead the following generalized asymptotic expansion (see §3.1): for any $\ell \in \mathbb{N}$, we have as $n \rightarrow +\infty$

$$\gamma_\ell \sim \sum_{j=1}^{n-1} \frac{\ln^\ell(j)}{j} + \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell+1} - \sum_{k=0}^{\ell} \frac{\ell! \ln^{\ell-k}(n)}{(\ell-k)!} \sum_{m=0}^{\infty} \frac{1}{n^{2m+2}} \frac{B_{2m+2}}{(2m+2)!} S(2m+2, k+1), \quad (4)$$

where the $S(n, k)$ are Stirling's numbers of the first kind defined by $x(x-1)\cdots(x-n+1) = \sum_{k=0}^n S(n, k)x^k$. Let us define the formal power series $\Phi_k(z)$, $k \in \mathbb{N}$, by

$$\Phi_k(z) := \sum_{m=0}^{\infty} \frac{(-1)^{m+1} B_{2m+2}}{(2m+2)!} S(2m+2, k+1) z^m.$$

The central point of the paper is to replace the asymptotic series $\Phi_k(-1/n^2)$ in (4) by some Padé type approximants and not by some Padé approximants as in our previous papers. The basic properties of Padé type approximants are recalled in Section 2 and below $(\mu/\nu)_f(z)$ denotes the Padé type approximant of $f(z)$ with numerator and denominator of degree $\leq \mu$ and $\leq \nu$ respectively. The denominator is a specified polynomial of degree ν and the numerator is then determined such that the Taylor expansion of the rational fraction matches the Taylor expansion of $f(z)$ up to z^μ at $z = 0$. We shall consider the polynomial

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

as the generating polynomial (see §2) for the denominators of the Padé type approximants $(rn + p/rn)_{\Phi_k}$, where $\alpha := p + 4$. It is a special case of Wilson polynomials [11]; see §4 for details. Note that the definition of $T_{rn}(\alpha, x)$ is independent of the choice of the sign \pm ; we will take advantage of this fact in §6.

Theorem 1. *Let $r \in \mathbb{Q}_{\geq 0}$ be such that $rn \in \mathbb{N}$. Define $\mu_r := \frac{2r}{r+\sqrt{1+r^2}}$. Then for every integers $n \geq 1$ and $p \geq \ell/2$,*

$$\gamma_\ell = \sum_{j=1}^n \frac{\ln^\ell(j)}{j} - \frac{\ln^{\ell+1}(n)}{\ell+1} - \frac{\ln^\ell(n)}{2n} + \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell-k)!} (rn + p/rn)_{\Phi_k}(-1/n^2) + \delta_{rn,p,\ell} \quad (5)$$

where

$$\limsup_{n \rightarrow +\infty, rn \in \mathbb{N}} |\delta_{rn,p,\ell}|^{1/n} \leq \left(\frac{2r - \mu_r}{2r + \mu_r} \right)^{2r} (1 - \mu_r) < 1.$$

Remark. Even though this is not the point of view of the present paper (which remains at a theoretical level because no complexity analysis was performed), it could be interesting to compare the algorithms obtained in [1, 5] for the high precision computation of Stieltjes' constants with the one that could be obtained from Theorem 1.

We presented Corollary 2 in [9] as an effective version of Stirling's formula. It is also possible to view this corollary in a dual way as an approximation of $\log \sqrt{2\pi}$ in the spirit of Theorem 1 above:

$$\log \sqrt{2\pi} = \ln(n!) - n \ln(n) + n - \frac{1}{2} \ln(n) - \frac{1}{12n} + \frac{1}{n^3} [rn - 1/rn]_{\Omega}(-1/n^2) + \widehat{\delta}_{r,n}.$$

where $\limsup_{n \rightarrow +\infty, rn \in \mathbb{N}} |\widehat{\delta}_{r,n}|^{1/n} \leq (r/2e)^{4r}$ and $\Omega(z) := -\sum_{n=0}^{\infty} (-z)^n B_{2n+4} / ((2n+4)(2n+3))$ is a formal series similar to $\widehat{\Phi}$.

The paper is organized as follows. In §2, we recall the definition of Padé type approximant and the important formula of the error. In §3, we collect various results needed for the proof of Theorem 1, in particular a moment interpretation of the coefficients of Φ_k involving some explicit weight functions w_k , for which we find an upper bound in term of Wilson weight. The properties of the latter are recalled in §4. Theorem 1 is proved in §5. In §6, we provide explicit expression of the Padé type approximants in Theorem 1. Finally, we refine our method for Stieltjes' constant γ_1 in §7 (Theorem 2) and we also apply it to the Riemann zeta function in §8 (Theorem 3).

2. PADÉ TYPE APPROXIMANTS

In this section, we remind the definition and basic properties of *Padé type approximants*. See [6, Chapter 1] for more details.

Let V_n be a polynomial of degree n and $f(z) = \int_0^{\infty} \frac{\mu(x)}{1-zx} dx$ where the weight function $\mu(x)$ is not necessarily positive on $[0, +\infty)$ and is such that $\int_0^{\infty} x^n |\mu(x)| dx < \infty$ for all integer $n \geq 0$. V_n will be called the *generating polynomial* of the Padé type approximant. Let W_{n-1} be the associated polynomial of V_n with respect to the weight μ : by definition,

$$W_{n-1}(z) := \int_0^{\infty} \frac{V_n(x) - V_n(z)}{x - z} \mu(x) dx.$$

and it is of degree $\leq n - 1$.

We set $\widetilde{W}_{n-1}(z) := z^{n-1} W_{n-1}(1/z)$ and $\widetilde{V}_n(z) := z^n V_n(1/z)$, so that

$$\begin{aligned} f(z) - \frac{\widetilde{W}_{n-1}(z)}{\widetilde{V}_n(z)} &= \int_0^{\infty} \frac{\mu(x)}{1-zx} dx - \frac{z^{-1}}{V(z^{-1})} \int_0^{\infty} \frac{V(x) - V(z^{-1})}{x - z^{-1}} \mu(x) dx \\ &= \int_0^{\infty} \frac{\mu(x)}{1-zx} dx + \int_0^{\infty} \frac{V_n(x)/V_n(z^{-1}) - 1}{1-zx} \mu(x) dx \\ &= \frac{z^n}{\widetilde{V}_n(z)} \int_0^{\infty} \frac{V_n(x)}{1-zx} \mu(x) dx. \end{aligned} \tag{6}$$

Thus, the Taylor expansion at $z = 0$ of the rational fraction $\widetilde{W}_{n-1}(z)/\widetilde{V}_n(z)$ coincides with that of $f(z)$ up to z^{n-1} at $z = 0$. By analogy with Padé approximant, the quotient $\frac{\widetilde{W}_{n-1}(z)}{\widetilde{V}_n(z)}$ is denoted $(n-1/n)_f(z)$ and is called a Padé type approximant to $f(z)$. Note that if V_n is orthogonal with respect to μ (ie $\int_0^\infty x^k V_n(x) \mu(x) dx = 0$ for $0 \leq k \leq n-1$), we can replace in (6) V_n and \widetilde{V}_n by their square respectively, and z^n by z^{2n} so that the error is $O(z^{2n})$.

More generally, we define

$$(n+p-1/n)_f := c_0 + c_1 z + c_2 z^2 + \cdots + c_{p-1} z^{p-1} + z^p (n-1/n)_{f_p}$$

where $p \in \mathbb{N}$ and $f_p(z) := c_p + c_{p+1} z + \cdots$. This means that the weight μ is thus multiplied by x^p . The error $f(z) - (n+p-1/n)_f(z)$ then satisfies

$$f(z) - (n+p-1/n)_f(z) = \frac{z^{p+n}}{\widetilde{V}_n(z^{-1})} \int_0^\infty \frac{V_n(x)}{1-xz} x^p \mu(x) dx. \quad (7)$$

3. AUXILIARY RESULTS

In this section, we collect and prove various results that will be used in the proof of Theorem 1.

3.1. Proof of the asymptotic expansion (4). If $\ell = 0$, then $S(2m+2, 1) = -(2m+1)!$. Hence (4) is a generalization of (1). Israilov proved in [7] that, when $n \rightarrow +\infty$,

$$\begin{aligned} \gamma_\ell = & \sum_{k=1}^n \frac{\ln^\ell(k)}{k} - \frac{\ln^{\ell+1}(n)}{\ell+1} - \frac{\ln^\ell(n)}{2n} \\ & - \sum_{k=1}^{N-1} \frac{B_{2k}}{(2k)!} \left(\frac{\log^\ell(x)}{x} \right)_{|x=n}^{(2k-1)} - \frac{\theta \cdot B_{2N}}{(2N)!} \left(\frac{\log^\ell(x)}{x} \right)_{|x=n}^{(2N-1)}, \end{aligned}$$

where $0 < \theta < 1$. Now, we have

$$\left(\frac{\log^\ell(x)}{x} \right)^{(p)} = \frac{\ell!}{x^{p+1}} \sum_{j=1}^{\ell+1} \frac{S(p+1, j)}{(\ell-j+1)!} \log^{\ell-j+1}(x).$$

After rearrangement, we then obtain the asymptotic expansion (4) as $n \rightarrow +\infty$.

3.2. An integral representation. Using formula (3) and its asymptotic expansion (4), we are now in position to obtain an integral representation for the coefficients in (4).

Proposition 1. *For every integers $m \geq 0$, $k \geq 0$, we have*

$$\frac{(-1)^{m+1} B_{2m+2}}{(2m+2)!} S(2m+2, k+1) = \int_0^\infty x^{2m} w_k(x) dx, \quad (8)$$

where the weight function w_k is defined by

$$w_k(x) := \frac{ix}{\pi(k+1)!} \int_x^\infty \left(\left(\log\left(\frac{y}{x} - 1\right) + i\pi \right)^{k+1} - \left(\log\left(\frac{y}{x} - 1\right) - i\pi \right)^{k+1} \right) \frac{d}{dy} \cdot \left(\frac{1}{e^{2\pi y} - 1} \right) dy.$$

Remarks. An equivalent expression is given by

$$w_k(x) = \frac{-2x}{(k+1)!} \sum_{q=0}^{k/2} \binom{k+1}{2q+1} (-\pi^2)^q \int_x^\infty \log^{k-2q}\left(\frac{y}{x} - 1\right) \cdot \frac{d}{dy} \left(\frac{1}{e^{2\pi y} - 1} \right) dy.$$

For $m = 0$ and $k \geq 2$, $\int_0^\infty w_k(x) dx = 0$ because $S(2, k+1) = 0$. Therefore, none of the weight functions w_k can have a constant sign on $[0, +\infty)$ when $k \geq 2$.

We first need a lemma

Lemma 1. For every real numbers $a > 0, t \geq 0$ and every integer $k \geq 0$, we have

$$\int_0^t \left| \frac{x}{a^2 + x^2} (\log a(t/x - 1) + i\pi)^k \right| dx \leq D \cdot C^k (k+1)! t^2$$

for some constants $C, D > 0$ that depend on a but neither on k nor t .

Proof. We have

$$\begin{aligned} I &:= \int_0^t \left| \frac{x}{a^2 + x^2} (\log a(t/x - 1) + i\pi)^k \right| dx \\ &\leq \frac{1}{a^2} \sum_{n=0}^k \binom{k}{n} (|\log(a)| + \pi)^{k-n} \int_0^t x |\log(t/x - 1)|^n dx \\ &\leq \frac{t}{a^2} 2^k (|\log(a)| + \pi)^k \sum_{n=0}^k \int_0^t |\log(t/x - 1)|^n dx. \end{aligned}$$

Now,

$$\begin{aligned} \int_0^t |\log(t/x - 1)|^n dx &\stackrel{u=t/x-1}{=} t \int_0^\infty \frac{|\log(u)|^n}{(1+u)^2} du \\ &= 2t \int_0^1 \frac{\log^n(1/u)}{(1+u)^2} du \leq 2t \int_0^1 \log^n(1/u) = 2tn!. \end{aligned}$$

Therefore,

$$0 \leq I \leq \frac{2^{k+1} (|\log(a)| + \pi)^k}{a^2} t^2 \sum_{n=0}^k n! \leq D \cdot C^k (k+1)! t^2$$

with $D := 2/a^2$ and $C := 2(|\log(a)| + \pi)$. □

Proof of Proposition 1. In [8], the first named author proved the following formula for the Hurwitz zeta function: for any complex numbers s, a such that $\Re(s) > 0, \Re(a) > 0$, and any positive integer $m > \Re(s) - 1$, we have

$$\zeta(s, a) = \frac{1}{a^{s-1}} \left(\frac{1}{s-1} + \frac{1}{2a} + \int_0^\infty \frac{1}{a^2 + x^2} \nu_s(x) dx \right) \quad (9)$$

where

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

If s is such that $\Re(s) < 2$ (in particular if s is “close to” 1), we can take $m = 1$ and thus

$$a^{1-s} \nu_s(x) = \frac{-2x^s a^{1-s} \sin(\pi s)}{(1-s)\pi} \int_x^\infty (t-x)^{1-s} \cdot \frac{d}{dt} \left(\frac{1}{e^{2\pi t} - 1} \right) dt. \quad (10)$$

For ease of reading, we set $\varphi(t) := \frac{d}{dt} \left(\frac{1}{e^{2\pi t} - 1} \right) = -\frac{2\pi e^{2\pi t}}{(e^{2\pi t} - 1)^2}$ in the rest of this section.

We now assume that $a > 0, t, x \in \mathbb{R}$ and that $t \geq x$. The Laurent expansion of $\frac{-2x^s a^{1-s} \sin(\pi s)}{(1-s)\pi} (t-x)^{1-s}$ at $s = 1$ is

$$\frac{-2x^s a^{1-s} \sin(\pi s)}{(1-s)\pi} (t-x)^{1-s} = \frac{-2x}{\pi} \Im \sum_{k=1}^\infty \frac{(1-s)^{k-1}}{k!} (\ln a(t/x - 1) + i\pi)^k. \quad (11)$$

The series starts at $k = 1$ and not $k = 0$ because the left-hand side is holomorphic at $s = 1$; the series converges for all $s \in \mathbb{C}$. By Lemma 1, we deduce that, for s close enough to 1, the series

$$\sum_{k=1}^\infty \frac{|s-1|^{k-1}}{k!} \int_0^\infty |\varphi(t)| \int_0^t \left| \frac{x}{a^2 + x^2} (\log(a(t/x - 1) + i\pi)^k) \right| dx dt$$

converges. Therefore, for s close to 1 (which depends on the value of a), we can exchange the various integrals and series when we use (9) and (10) in conjunction with (11), and this provides the Laurent series expansion of $\zeta(s, a)$ at $s = 1$. Since for $\ell \geq 0$, $(-1)^\ell \frac{\gamma_\ell(a)}{\ell!}$ is the coefficient of $(s-1)^\ell$ in the Laurent series expansion of $\zeta(s, a)$ at $s = 1$, unicity of such expansion yields, for all $\ell \geq 0$ and all $a > 0$,

$$\begin{aligned} \gamma_\ell(a) &= \frac{\log^\ell(a)}{2a} - \frac{\log^{\ell+1}(a)}{\ell+1} \\ &\quad + \frac{2(-1)^\ell}{\pi(\ell+1)} \Im \int_0^\infty \frac{x}{a^2 + x^2} \int_x^\infty (\log a(t/x - 1) + i\pi)^{\ell+1} \varphi(t) dt dx. \end{aligned} \quad (12)$$

We shall now compute the asymptotic expansion of the right-hand side of the previous identity for $\gamma_\ell(a)$ when $a \rightarrow +\infty$ (recall that $a \in (0, +\infty)$). We first observe that for every integers $k, p \geq 0$, the function

$$(t, x) \mapsto x^{2k+1} |\ln^p(t/x - 1) \varphi(t)| 1_{\{0 \leq x \leq t\}}(t, x)$$

is integrable on $[0, +\infty) \times [0, +\infty)$. Therefore, the following computations are licit: for any integer $k \geq 0$, we have

$$\begin{aligned}
& \int_0^\infty \frac{x}{a^2 + x^2} \int_x^\infty (\log a(t/x - 1) + i\pi)^{\ell+1} \varphi(t) dt dx \\
&= \sum_{m=0}^{k-1} \frac{(-1)^m}{a^{2m+2}} \int_0^\infty x^{2m+1} \int_x^\infty (\log a(t/x - 1) + i\pi)^{\ell+1} \varphi(t) dt dx \\
&\quad + \int_0^\infty \frac{(-1)^k x^{2k+1}}{a^{2k}(a^2 + x^2)} \int_x^\infty (\log a(t/x - 1) + i\pi)^{\ell+1} \varphi(t) dt dx \\
&= \sum_{m=0}^{k-1} \frac{(-1)^m}{a^{2m+2}} \int_0^\infty x^{2m+1} \int_x^\infty (\log a(t/x - 1) + i\pi)^{\ell+1} \varphi(t) dt dx + \mathcal{O}(a^{-2k-2}),
\end{aligned}$$

where in the last line $a \rightarrow +\infty$ and the implicit constant in \mathcal{O} depends on k .

Using (12) with $a = n$, the generalized asymptotic expansion of $\gamma_\ell(n)$ as $n \rightarrow +\infty$ is thus

$$\begin{aligned}
\gamma_\ell(n) &\sim \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell+1} \\
&\quad + \frac{2}{\pi(\ell+1)} \sum_{m=0}^{\infty} \frac{(-1)^m}{n^{2m+2}} \int_0^\infty x^{2m+1} \int_x^\infty \Im((\ln n(t/x - 1) + i\pi)^{\ell+1}) \varphi(t) dt dx.
\end{aligned}$$

Comparing this expression and Eq. (4) (stated in the introduction), unicity of such an asymptotic expansion implies that for any integers $k, m \geq 0$, we have

$$\begin{aligned}
& (-1)^{m+1} \frac{B_{2m+2}}{(2m+2)!} S(2m+2, k+1) \\
&= \frac{-2}{\pi(k+1)!} \int_0^\infty x^{2m+1} \int_x^\infty \Im((\ln(t/x - 1) + i\pi)^{k+1}) \varphi(t) dt dx.
\end{aligned}$$

This completes the proof of Proposition 1. \square

3.3. Bounds for the weights $w_k(x)$. To choose the generating polynomial of the Padé type approximant, we shall first find an upper bound of the weight w_k in term of a weight function of which we know explicite the orthogonal polynomials.

The goal of this section is to prove the following

Proposition 2. *For any integers k, p such that and $0 \leq k \leq 2p$, and for any $x \geq 0$, the weight function*

$$w_k(x) := \frac{-2x}{(k+1)!} \sum_{q=0}^{k/2} \binom{k+1}{2q+1} (-\pi^2)^q \int_x^\infty \ln^{k-2q}(y/x - 1) \frac{d}{dy} \left(\frac{1}{e^{2\pi y} - 1} \right) dy$$

satisfies

$$x^{2p+1} |w_k(x)| \leq 8 \sinh(\pi) G(p+4, 1, x),$$

where

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

We need the following lemma.

Lemma 2. *For every $x \geq 0$ and every integer $p \geq 0$,*

$$e^{-2\pi x} \frac{x^2}{(1 - e^{-2\pi x})^2} (1 + x^2)^{p+1/2} \leq G(p + 4, 1, x).$$

Proof. First, let us remark that for $\alpha \in \mathbb{R}$, $G(\alpha + 1, 1, x) = (\alpha^2 + x^2)G(\alpha, 1, x)$. In [10], we proved that for every $x \geq 0$ and every integer $m \geq 0$, we have $e^{-2\pi x} \leq G(1, 1, x)$ and

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

Hence,

$$\begin{aligned} \frac{x^2 (1 + x^2)^{p+1/2} e^{-2\pi x}}{(1 - e^{-2\pi x})^2} &\leq \frac{x^2}{(1 - e^{-2\pi x})^2} (1 + x^2)^{p+1/2} G(2, 1, x) \\ &\leq (x^2 + 1)^{p+1/2} G(3, 1, x) \leq G(p + 4, 1, x). \end{aligned}$$

□

Proof of Proposition 2. Using Proposition 1, we see that

$$|w_k(x)| \leq \frac{2x}{(k+1)!} \sum_{q=0}^{k/2} \binom{k+1}{2q+1} \pi^{2q} \int_x^\infty |\ln^{k-2q}(y/x - 1)| \frac{2\pi e^{2\pi y}}{(e^{2\pi y} - 1)^2} dy.$$

Note that $\binom{k+1}{2q+1} = 0$ if $q = (k+1)/2$, hence the sum stops at $q = k/2$ (at most). We split the interval $[x, \infty[$ into two intervals $[x, 2x]$ and $[2x, +\infty)$, on which the function $y \mapsto \ln(y/x - 1)$ has a constant sign.

Let us first consider the integral $\int_x^{2x} |\ln^{k-2q}(y/x - 1)| \frac{2\pi e^{2\pi y}}{(e^{2\pi y} - 1)^2} dy$:

$$\begin{aligned} \int_x^{2x} |\ln^{k-2q}(y/x - 1)| \frac{2\pi e^{2\pi y}}{(e^{2\pi y} - 1)^2} dy &\leq (-1)^{k-2q} \frac{2\pi e^{2\pi x}}{(e^{2\pi x} - 1)^2} \int_x^{2x} \ln^{k-2q}(y/x - 1) dy \\ &= (-1)^{k-2q} \frac{2\pi e^{2\pi x} x}{(e^{2\pi x} - 1)^2} \int_0^1 \ln^{k-2q}(u) du \\ &= \frac{2\pi e^{2\pi x} x}{(e^{2\pi x} - 1)^2} (k - 2q)!. \end{aligned}$$

The second integral is treated as follows:

$$\begin{aligned}
\int_{2x}^{\infty} \frac{2\pi |\ln^{k-2q}(y/x-1)|}{(e^{\pi y} - e^{-\pi y})^2} dy &\leq \frac{2\pi}{(1 - e^{-4\pi x})^2} \int_{2x}^{\infty} \ln^{k-2q}(y/x-1) e^{-2\pi y} dy \\
&= \frac{2\pi(k-2q)}{(1 - e^{-4\pi x})^2} \int_{2x}^{\infty} \frac{1}{y-x} \ln^{k-2q-1}(y/x-1) \frac{e^{-2\pi y}}{2\pi} dy \\
&\leq \frac{2\pi(k-2q)}{(1 - e^{-4\pi x})^2} \frac{1}{x} \int_{2x}^{\infty} \ln^{k-2q-1}(y/x-1) \frac{e^{-2\pi y}}{2\pi} dy \\
&\leq \frac{2\pi(k-2q)!}{(1 - e^{-4\pi x})^2} \frac{1}{x^{k-2q}} \int_{2x}^{\infty} \frac{e^{-2\pi y}}{(2\pi)^{k-2q}} dy \\
&= \frac{(k-2q)!}{(1 - e^{-4\pi x})^2} \frac{e^{-4\pi x}}{(2\pi x)^{k-2q}}
\end{aligned}$$

(after $k-2q$ integrations by parts).

Therefore

$$\begin{aligned}
|w_k(x)| &\leq 2x \sum_{q=0}^{k/2} \frac{\pi^{2p}}{(2q+1)!} \left(\frac{2\pi x e^{2\pi x}}{(e^{2\pi x} - 1)^2} + \frac{1}{(1 - e^{-4\pi x})^2} \frac{e^{-4\pi x}}{(2\pi x)^{k-2p}} \right) \\
&= 2x \sum_{q=0}^{k/2} \frac{\pi^{2q} e^{-2\pi x}}{(2q+1)!} \left(\frac{2\pi x}{(1 - e^{-2\pi x})^2} + \frac{1}{(1 - e^{-4\pi x})^2} \frac{1}{(2\pi x)^{k-2q}} \right) \\
&\leq 2x \sum_{q=0}^{k/2} \frac{\pi^{2q} e^{-2\pi x}}{(2q+1)!} \frac{2\pi x}{(1 - e^{-2\pi x})^2} \left(1 + (2\pi x)^{-k+2q-1} \right).
\end{aligned}$$

It follows that

$$\begin{aligned}
x^{2p+1} |w_k(x)| &\leq 4x^2 \sum_{q=0}^{k/2} \frac{\pi^{2q+1} e^{-2\pi x} (x^{2p+1} + x^{2p-k+2q})}{(2q+1)! (1 - e^{-2\pi x})^2} \\
&\leq \frac{8x^2 (1+x^2)^{(2p+1)/2} e^{-2\pi x}}{(1 - e^{-2\pi x})^2} \sum_{q=0}^{k/2} \frac{\pi^{2q+1}}{(2q+1)!} \quad (\text{because } x \leq (1+x^2)^{1/2}) \\
&\leq e^{-2\pi x} \frac{8x^2 (1+x^2)^{(2p+1)/2}}{(1 - e^{-2\pi x})^2} \sum_{q=0}^{k/2} \frac{\pi^{2q+1}}{(2q+1)!} \\
&\leq 8G(p+4, 1, x) \sum_{q=0}^{\infty} \frac{\pi^{2q+1}}{(2q+1)!} \quad (\text{by Lemma 2}) \\
&= 8 \sinh(\pi) G(p+4, 1, x).
\end{aligned}$$

This completes the proof of Proposition 2. □

4. A REVIEW OF WILSON'S POLYNOMIALS PROPERTIES

To proceed further, we make a crucial observation: the function $G(\alpha, \beta, x)$ considered in Proposition 2 is Wilson's weight on $(0, +\infty)$, for which the orthogonal polynomials are explicitly known; see [2, 11]. We review their properties 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

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

In particular, for all integer $n \geq 0$,

$$\int_0^{+\infty} T_n^2(\alpha, \beta, x) \gamma(\alpha, \beta, x) dx = \frac{\pi^2 (4n + 2\alpha + 2\beta - 1) (2n)! \Gamma(2n + 2\alpha) \Gamma(2n + 2\beta) \Gamma(2n + 2\alpha + 2\beta - 1)}{2^{8n+4\alpha+4\beta-3} \Gamma(2n + \alpha + \beta + \frac{1}{2})^2}. \quad (13)$$

If $\beta = 1$, then

$$T_n(\alpha, 1, x) = \frac{(-1)^n (2n)! (\alpha)_{2n+1}}{(2n + 2\alpha)_{2n+1}} \sum_{j=0}^{2n} \binom{2n+1}{j+1} \binom{2n+2\alpha+j}{j+1} \binom{i\sqrt{x}-1}{j} / \binom{\alpha+j}{j+1} \quad (14)$$

and, after simplification of (13), we obtain

$$\int_0^{+\infty} T_n^2(\alpha, 1, x) \gamma(\alpha, 1, x) dx = \frac{2\pi(2n+2\alpha)}{(2n+1)(4n+2\alpha+1)} \frac{\Gamma(2n+\alpha+1)^2}{\binom{4n+2\alpha}{2n+1}} \quad (15)$$

and

$$\int_0^{+\infty} \gamma(\alpha, 1, x) dx = \frac{\pi\alpha}{(2\alpha+1)} \Gamma(\alpha)^2. \quad (16)$$

5. PROOF OF THEOREM 1

We define

$$\Psi_k(z) = \int_0^\infty \frac{w_k(x)}{1-zx^2} dx = \int_0^\infty \frac{1}{1-zx} \frac{w_k(\sqrt{x})}{2\sqrt{x}} dx, \quad z \in \mathbb{C} \setminus [0, +\infty).$$

Proposition 1 implies that as $z \rightarrow 0$ in any angular open sector that does not contain $[0, +\infty)$, the asymptotic expansion of $\Psi_k(z)$ is given by $\Phi_k(z)$. (See [9, §2] for more details in a very similar situation).

From the results proved in §3, it is immediate that Eqs. (2) and (12) (with $a = n$) imply that for every integer $n \geq 1$,

$$\gamma_\ell = \sum_{j=1}^n \frac{\ln^\ell(j)}{j} - \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell+1} + \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell-k)!} \Psi_k\left(-\frac{1}{n^2}\right). \quad (17)$$

5.1. A bound for the Padé type approximants of Φ_k . In this section, we shall prove the following bound, where we now make our choice for the generating polynomial of the Padé type approximants: we take $V_n(x) = T_n(\alpha, 1, x)$, which we shall simplify as $T_n(\alpha, x)$ in the sequel.

Proposition 3. *Let $z \in \mathbb{C}$ such that $\Re(z) < 0$, and $s > 0$. For any integers $p \geq \ell/2$ and $k \geq 0$, set $\varepsilon_{n,p,k}(z) := \Psi_k(z) - (n+p/n)\Phi_k(z)$. Then,*

$$|\varepsilon_{n,p,k}(z)| \leq \varepsilon_{n,p}(z) := C \frac{|z|^{p+1}}{|T_n(\alpha, z^{-1})|} \frac{\Gamma(2n+\alpha+1)}{\binom{4n+2\alpha}{2n+1}} \left(\frac{(2n+2\alpha)}{(2n+1)(4n+2\alpha+1)} \right)^{1/2}, \quad (18)$$

where $\alpha := p+4$ and $C := 4\pi \sinh(\pi) \Gamma(\alpha+1) \left(\frac{2\alpha}{2\alpha+1}\right)^{1/2}$.

Proof. The difference between the function Ψ_k and its Padé type approximant is

$$\Psi_k(z) - (n+p/n)\Phi_k(z) = \frac{z^{p+1}}{T_n(\alpha, z^{-1})} \int_0^\infty x^{p+1} \frac{w_k(\sqrt{x})}{2\sqrt{x}} \frac{T_n(\alpha, 1, x)}{1-zx} dx.$$

(See (7) in §2.) Hence, using Proposition 2, the Cauchy-Schwartz inequality, (15) and (16), we have that

$$\begin{aligned}
|\varepsilon_{n,p,k}(z)| &\leq \left| \frac{z^{p+1}}{T_n(\alpha, 1, z^{-1})} \right| \int_0^\infty \frac{|T_n(\alpha, 1, x)|}{|1-zx|} x^{p+1} |w_k(\sqrt{x})| \frac{1}{2\sqrt{x}} dx \\
&\leq \left| \frac{z^{p+1}}{T_n(\alpha, z^{-1})} \right| \int_0^\infty |T_n(\alpha, x)| x^{p+1} |w_k(\sqrt{x})| \frac{1}{2\sqrt{x}} dx \\
&\leq 4 \sinh \pi \left| \frac{z^{p+1}}{T_n(\alpha, z^{-1})} \right| \int_0^\infty |T_n(\alpha, x)| \gamma(\alpha, 1, x) dx \\
&\leq 4 \sinh \pi \left| \frac{z^{p+1}}{T_n(\alpha, z^{-1})} \right| \left(\int_0^\infty |T_n(\alpha, x)|^2 \gamma(\alpha, 1, x) dx \right)^{1/2} \left(\int_0^\infty \gamma(\alpha, 1, x) dx \right)^{1/2} \\
&\leq 4\pi \sinh \pi \left| \frac{z^{p+1}}{T_n(\alpha, z^{-1})} \right| \frac{\Gamma(2n + \alpha + 1)\Gamma(\alpha + 1)}{\binom{4n+2\alpha}{2n+1}} \left(\frac{2\alpha(2n + 2\alpha)}{(2n + 1)(4n + 2\alpha + 1)(2\alpha + 1)} \right)^{1/2}.
\end{aligned}$$

This completes the proof of Proposition 2. \square

5.2. Completion of the proof of Theorem 1. In Eq. (17), we want to replace $\Psi_k(-1/n^2)$ by the Padé type approximants $(rn + p/rn)_{\Phi_k}(-1/n^2)$ (for $p \geq \ell/2$) considered in §5.1. With the notations used in that section, we have

$$\begin{aligned}
\gamma_\ell &= \sum_{j=1}^n \frac{\ln^\ell(j)}{j} - \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell + 1} + \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell - k)!} (rn + p/rn)_{\Phi_k}(-1/n^2) \\
&\quad + \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell - k)!} \varepsilon_{rn,p,k}(-1/n^2) \\
&= \sum_{j=1}^n \frac{\ln^\ell(j)}{j} - \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell + 1} + \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell - k)!} (rn + p/rn)_{\Phi_k}(-1/n^2) + \delta_{rn,p,\ell},
\end{aligned}$$

where

$$\delta_{rn,p,\ell} = \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell - k)!} \varepsilon_{rn,p,k}(-1/n^2).$$

Then by Proposition 2, it follows that

$$|\delta_{rn,p,\ell}| \leq \frac{\ell!}{n^2} \varepsilon_{rn,p}(-1/n^2) \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell - k)!} \leq \frac{\ell!}{n} \varepsilon_{rn,p}(-1/n^2).$$

Now, by (18),

$$\begin{aligned} & \varepsilon_{rn,p}(-1/n^2) \\ &= 4\pi \sinh \pi \left| \frac{(-1/n^2)^{p+1}}{T_{rn}(\alpha, -n^2)} \right| \frac{\Gamma(2rn+\alpha+1)\Gamma(\alpha+1)}{\binom{4rn+2\alpha}{2rn+1}} \left(\frac{2\alpha(2rn+2\alpha)}{(2rn+1)(4rn+2\alpha+1)(2\alpha+1)} \right)^{1/2}. \end{aligned} \quad (19)$$

To compute $\limsup_n |\delta_{rn,p,\ell}|^{1/n}$ as $n \rightarrow +\infty$, the previous bound shows it is enough to compute $\limsup_n |\varepsilon_{rn,p}(-1/n^2)|^{1/n}$. For this, let us consider

$$\begin{aligned} \mathcal{T}_{rn}(\alpha, -n^2) &:= \frac{(-1)^{rn}(2rn+2\alpha)_{2rn+1}}{(2rn)!(\alpha)_{2rn+1}} T_{rn}(\alpha, -n^2) \\ &= \sum_{j=0}^{2rn} \binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1} \binom{n-1}{j} / \binom{\alpha+j}{j+1}. \end{aligned} \quad (20)$$

All the terms of this sum are positive and are zero when $j \geq \min(n, 2rn+1)$ because of the vanishing of the binomial coefficients $\binom{2rn+1}{j+1}$ and $\binom{n-1}{j}$. Applying Stirling's formula to the summand of $\mathcal{T}_{rn}(\alpha, -n^2)$, the discrete Laplace method (see [3, proof of Lemme 3]) implies that

$$\begin{aligned} \lim_{n \rightarrow \infty} \mathcal{T}_{rn}(\alpha, -n^2)^{1/n} &= \max_{0 \leq t \leq \min(1, 2r)} \frac{(2r+t)^{2r+t}}{t^{3t}(2r-t)^{2r-t}(1-t)^{1-t}} \\ &= \frac{(2r+\mu_r)^{2r}}{(2r-\mu_r)^{2r}(1-\mu_r)}, \end{aligned}$$

where $\mu_r = \frac{2r}{r+\sqrt{1+r^2}} < \min(1, 2r)$ is a root of $(1-t)(4r^2-t^2) = t^3$. After some simplifications of the term $\frac{(2rn+2\alpha)_{2rn+1}}{(2rn)!(\alpha)_{2rn+1}}$ (in (20)) with the term $\Gamma(2rn+\alpha+1)\Gamma(\alpha+1)/\binom{4rn+2\alpha}{2rn+1}$ in (19), it follows that

$$\limsup_{n \rightarrow \infty, rn \in \mathbb{N}} |\delta_{rn,p,\ell}|^{1/n} \leq \frac{(2r-\mu_r)^{2r}}{(2r+\mu_r)^{2r}}(1-\mu_r) < 1.$$

This completes the proof of Theorem 1.

For example, if $r = 1$, for any integer ℓ and $p \geq \ell/2$, $\limsup_{n \rightarrow \infty} |\delta_{n,p,\ell}|^{1/n} \leq (\sqrt{2}-1)^4 \approx 0.02943$. For $r = 2$, $\limsup_{n \rightarrow \infty} |\delta_{2n,p,\ell}|^{1/n} \leq \frac{1}{16}(\sqrt{5}-1)^4(\sqrt{5}-2)^2 \approx 0.00813$.

6. EXPRESSION OF THE PADÉ TYPE APPROXIMANTS IN THEOREM 1

The purpose of this section is to make completely explicit the Padé type approximants for the functions Φ_k , $0 \leq k \leq \ell$ involved in Theorem 1.

For the sake of simplicity, we define a linear functional $\Omega^{(k)}$ acting on the space of polynomials by $\langle \Omega^{(k)}, x^m \rangle := \Omega_{m+p+1}^{(k)}$, where $p \geq -1$ is a fixed integer and the moments

$(\Omega_m^{(k)})_{m \in \mathbb{N}}$ are defined by

$$\Omega_m^{(k)} := \frac{(-1)^{m+1} B_{2m+2}}{(2m+2)!} S(2m+2, k+1) = \int_0^\infty x^{2m} w_k(x) dx.$$

We recall that we have chosen (up to a multiplicative factor)

$$\mathcal{T}_{rn}(\alpha, x) := \sum_{j=0}^{2rn} \binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1} \binom{\pm i\sqrt{x}-1}{j} / \binom{\alpha+j}{j+1}$$

as the generating polynomial of all the denominator of the Padé type approximants $(rn + p/rn)_{\Phi_k}$. The numerator of $(rn + p/rn)_{\Phi_k}$ depends on k and requires the computation of the associated polynomial of degree $rn - 1$

$$W_{rn-1}^{(k)}(z) = \left\langle \Omega^{(k)}, \frac{\mathcal{T}_{rn}(\alpha, x) - \mathcal{T}_{rn}(\alpha, z)}{x - z} \right\rangle.$$

By linearity, it is enough to compute $\Omega^{(k)}$ applied to the polynomial

$$\frac{\binom{\pm i\sqrt{x}-1}{j} - \binom{\pm i\sqrt{z}-1}{j}}{x - z}.$$

For this purpose, it is necessary to expand it on the canonical basis. Since we can choose either $+$ or $-$ in the definition of $\mathcal{T}_{rn}(\alpha, x)$, the latter can be viewed as the mean of the expression with a $+$ and of the expression with a $-$. Hence, it is convenient to first compute the associated of the following polynomial

$$\frac{\binom{i\sqrt{x}-1}{j} + \binom{-i\sqrt{x}-1}{j}}{2}.$$

We have

$$\begin{aligned} \frac{\binom{i\sqrt{x}-1}{j} + \binom{-i\sqrt{x}-1}{j}}{2} &= \frac{1}{2j!} \sum_{q=0}^j S(j+1, q+1) ((i\sqrt{x})^q + (-i\sqrt{x})^q) \\ &= \frac{1}{j!} \sum_{q=0}^{j/2} S(j+1, 2q+1) x^q (-1)^q \end{aligned}$$

Hence,

$$\begin{aligned} \left\langle \Omega^{(k)}, \frac{\binom{i\sqrt{x}-1}{j} + \binom{-i\sqrt{x}-1}{j} - \binom{i\sqrt{z}-1}{j} - \binom{-i\sqrt{z}-1}{j}}{2(x-z)} \right\rangle \\ = \frac{1}{j!} \sum_{q=0}^{j/2} S(j+1, 2q+1) (-1)^q \sum_{s=0}^{q-1} z^{q-1-s} \Omega_{s+p+1}^{(k)}. \end{aligned}$$

Therefore, the associated polynomial of $\mathcal{T}_{rn}(\alpha, x)$ with respect to $\Omega^{(k)}$ is

$$\begin{aligned} W_{rn-1}^{(k)}(z) &:= \left\langle \Omega^{(k)}, \frac{\mathcal{T}_{rn}(\alpha, x) - \mathcal{T}_{rn}(\alpha, z)}{x - z} \right\rangle \\ &= \sum_{j=0}^{2rn} \frac{\binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1}}{\binom{\alpha+j}{j+1}} \left\langle \Omega^{(k)}, \frac{\binom{i\sqrt{x}-1}{j} + \binom{-i\sqrt{x}-1}{j} - \binom{i\sqrt{z}-1}{j} - \binom{-i\sqrt{z}-1}{j}}{2(x-z)} \right\rangle \\ &= \sum_{j=0}^{2rn} \frac{\binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1}}{\binom{\alpha+j}{j+1}} \frac{1}{j!} \sum_{q=0}^{j/2} S(j+1, 2q+1) (-1)^q \sum_{s=0}^{q-1} z^{q-1-s} \Omega_{s+p+1}^{(k)}. \end{aligned}$$

The Padé type approximant $(rn + p/rn)_{\Phi_k}(z)$ is then

$$\sum_{j=0}^p \Omega_j^{(k)} z^j + \frac{z^p W_{rn-1}^{(k)}(z^{-1})}{\mathcal{T}_{rn}(\alpha, 1, z^{-1})}.$$

Hence, we have

$$\gamma_\ell = \sum_{j=1}^n \frac{\ln^\ell(j)}{j} - \frac{\ln^\ell(n)}{2n} - \frac{\ln^{\ell+1}(n)}{\ell+1} + \frac{\ell!}{n^2} \sum_{k=0}^{\ell} \frac{\ln^{\ell-k}(n)}{(\ell-k)!} (rn + p/rn)_{\Phi_k}(-1/n^2)$$

where

$$\begin{aligned} (rn + p/rn)_{\Phi_k}(-1/n^2) &= \left(\sum_{j=0}^p \Omega_j^{(k)} z^j + \frac{z^p W_{rn-1}^{(k)}(z^{-1})}{\mathcal{T}_{rn}(\alpha, z^{-1})} \right) \Big|_{z=-1/n^2} \\ &= \sum_{j=0}^p \Omega_j^{(k)} \left(\frac{-1}{n^2} \right)^j + \left(\frac{-1}{n^2} \right)^p \frac{N_k}{D} \end{aligned}$$

and

$$\begin{aligned} N_k &:= \sum_{j=0}^{2rn} \frac{\binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1}}{j! \binom{\alpha+j}{j+1}} \sum_{q=0}^{j/2} S(j+1, 2q+1) \sum_{s=0}^{q-1} (-1)^{s+1} n^{2q-2-2s} \Omega_{s+p+1}^{(k)} \\ D &:= \sum_{j=0}^{2rn} \binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1} \binom{n-1}{j} / \binom{\alpha+j}{j+1}, \end{aligned}$$

and $\alpha := p + 4$

7. THE PARTICULAR CASES $\ell = 0$ AND $\ell = 1$

The beginning of the paper deals with approximations of Stieltjes' constants in a general way, i.e. by adding to the partial sum of order n defining γ_ℓ the sum of a Padé type approximant to the asymptotic expansion of the remainder as a function of $1/n$. The reason for this approach is that the weight functions underlying this expansion do not have a constant sign on $[0, +\infty)$. However for $\ell = 0$ and $\ell = 1$, as we shall show, the weights w_0

and w_1 have a constant sign. As a consequence, we can use ordinary Padé approximants instead of Padé type approximants.

The case $\ell = 0$ has already been fully treated in [9]. In this case, for every $x > 0$,

$$w_0(x) = -2x \int_x^\infty \frac{d}{dy} \left(\frac{1}{e^{2\pi y} - 1} \right) dy = \frac{2x}{e^{2\pi x} - 1} \geq 0.$$

The case $\ell = 1$ is more complicated. We have, for every $x > 0$,

$$\begin{aligned} w_1(x) &= 4\pi x \int_x^\infty \ln(y/x - 1) \frac{e^{2\pi y}}{(e^{2\pi y} - 1)^2} dy \\ &= 4\pi x^2 \int_0^1 \ln(1/v - 1) \frac{e^{2\pi x/v}}{(e^{2\pi x/v} - 1)^2} \frac{dv}{v^2} \quad (v = x/y) \\ &= 4\pi x^2 \left(\int_0^1 \ln(1-v) \frac{e^{2\pi x/v}}{(e^{2\pi x/v} - 1)^2} \frac{dv}{v^2} - \int_0^1 \ln(v) \frac{e^{2\pi x/v}}{(e^{2\pi x/v} - 1)^2} \frac{dv}{v^2} \right) \\ &= 4\pi x^2 \left(\int_0^1 \ln(1-v) \frac{e^{2\pi x/v}}{(e^{2\pi x/v} - 1)^2} \frac{dv}{v^2} - \int_0^1 \ln(1-v) \frac{e^{2\pi x/(1-v)}}{(e^{2\pi x/(1-v)} - 1)^2} \frac{dv}{(1-v)^2} \right) \\ &= 4\pi x^2 \int_0^1 \ln(1-v) \Psi(v) dv \end{aligned}$$

where

$$\Psi(v) := \frac{e^{2\pi x/v}}{(e^{2\pi x/v} - 1)^2} \frac{1}{v^2} - \frac{e^{2\pi x/(1-v)}}{(e^{2\pi x/(1-v)} - 1)^2} \frac{1}{(1-v)^2}.$$

Because $y \mapsto \frac{1}{e^{2\pi y} - 1}$ is completely monotonic on $[0, +\infty)$, the function $\Psi(v)$ is increasing on $[0, 1]$ for any fixed x . Moreover it is an odd function around $v = 1/2$ and $\Psi(1/2) = 0$. Hence, Ψ is negative on $[0, 1/2]$, positive on $[1/2, 1]$ and $\int_0^1 \Psi(v) dv = 0$. Now, on $[0, 1/2]$, $\ln(1-v) \geq -\ln(2)$ and $\Psi(v) \leq 0$ so that $\ln(1-v)\Psi(v) \leq -\ln(2)\Psi(v)$, while on $[1/2, 1]$, $\ln(1-v) \leq -\ln(2)$ and $\Psi(v) \geq 0$ so that $\ln(1-v)\Psi(v) \leq -\ln(2)\Psi(v)$. Writing

$$w_1(x) = 4\pi x^2 \left(\int_0^{1/2} \ln(1-v) \Psi(v) dv + \int_{1/2}^1 \ln(1-v) \Psi(v) dv \right),$$

we deduce that

$$w_1(x) \leq -4\pi x^2 \ln(2) \int_0^1 \Psi(v) dv = 0,$$

and thus the weight function $w_1(x)$ has a constant sign on $[0, +\infty)$.

The approximation of γ_1 in terms of Padé approximants is thus

$$\sum_{j=1}^n \frac{\ln(j)}{j} - \frac{\ln(n)}{2n} - \frac{\ln^2(n)}{2} - [rn + p/rn]_{\Phi_1}(-1/n^2) - \ln(n) [rn + p/rn]_{\Phi_0}(-1/n^2)$$

for any integers $n, p \geq 1$ and any $r \in \mathbb{Q}_{\geq 0}$ such that $rn \in \mathbb{N}$. We display the error without any calculations. We have

$$\begin{aligned}\tilde{\varepsilon}_{rn,p}^{(0)}(z) &:= \Psi_0(z) - [rn + p/rn]_{\Phi_0}(z) = \frac{z^{p+1}}{(P_{rn}^{(0)}(\alpha, z^{-1}))^2} \int_0^\infty \frac{(P_{rn}^{(0)}(\alpha, x))^2 x^{p+1} w_0(\sqrt{x})}{1-zx} \frac{1}{2\sqrt{x}} dx, \\ \tilde{\varepsilon}_{rn,p}^{(1)}(z) &:= \Psi_1(z) - [rn + p/rn]_{\Phi_1}(z) = \frac{z^{p+1}}{(P_{rn}^{(1)}(\alpha, z^{-1}))^2} \int_0^\infty \frac{(P_{rn}^{(1)}(\alpha, x))^2 x^{p+1} w_1(\sqrt{x})}{1-zx} \frac{1}{2\sqrt{x}} dx,\end{aligned}$$

where $P_{rn}^{(0)}(\alpha, z^{-1})$ and $P_{rn}^{(1)}(\alpha, z^{-1})$ are orthogonal polynomials with respect to the weight function $x^{p+1} w_1(\sqrt{x}) \frac{1}{2\sqrt{x}}$. Explicit expressions of these polynomials are not known, but it is known that their roots lie on $[0, \infty)$. Similar computations than those done in [9] then show that for $r < 2e$ and $m \in \{0, 1\}$, we have

$$\limsup_{n \rightarrow \infty, rn \in \mathbb{N}} |\tilde{\varepsilon}_{rn,p}^{(m)}(-1/n^2)|^{1/n} \leq \left(\frac{r}{2e}\right)^{4r} < 1.$$

This proves the following

Theorem 2. *For any fixed $r \in \mathbb{Q}_{\geq 0}$ such that $r < 2e$, we have*

$$\begin{aligned}\limsup_{n \rightarrow \infty, rn \in \mathbb{N}} \left| \gamma_1 - \left(\sum_{j=1}^n \frac{\ln(j)}{j} - \frac{\ln(n)}{2n} - \frac{\ln^2(n)}{2} \right. \right. \\ \left. \left. - [rn + p/rn]_{\Phi_1}(-1/n^2) - \ln(n)[rn + p/rn]_{\Phi_0}(-1/n^2) \right) \right|^{1/n} \leq \left(\frac{r}{2e}\right)^{4r}.\end{aligned}$$

8. AN APPLICATION TO THE RIEMANN ZETA FUNCTION

We first recall the previous results established by the authors. In [8], the first named author proved that for any complex number s , $\Re(s) > -1$ and any positive integer m , $m > \Re(s) - 1$, then

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} + \int_0^\infty \frac{1}{1+x^2} \nu_s(x) dx$$

where the weight function $\nu_s(x)$ is defined by:

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

As a consequence, he obtained an approximation of $\zeta(s)$ as follows. Let us define the formal power series

$$\tilde{\Psi}_s(t) := \sum_{k=0}^\infty \frac{B_k}{k!} (s)_{k-1} (-t)^k,$$

where $(s)_j$ is Pochhammer's symbol for $j \geq 0$ and $(s)_{-1} := \frac{1}{s-1}$. Then, using Carleman criteria, for all integer $p \geq 1$ and $s > 0, s \neq 1$, he proved that

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + (n+1)^{1-s} \lim_{m \rightarrow \infty} [m + p/m]_{\tilde{\Psi}}(1/(n+1)).$$

Note that n is fixed. The proof is based on the non-negativity of $\nu_s(x)$ on $[0, +\infty)$. Moreover, in [10], the two authors proved the following result: let $r \in \mathbb{Q}$ be such that $0 < r < 2e$ and $s > 0, s \neq 1$ and

$$\Theta_s(t) := \sum_{k \geq 0} \frac{B_{2k+2}}{(2k+2)!} (s)_{2k+1} (-t)^k = t^{-2} \left(\frac{-1}{s-1} + \frac{t}{2} + \tilde{\Psi}_s(t) \right).$$

Then, for every integer $n \geq 1$ such that rn is an integer, we have

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{(s-1)n^{s-1}} - \frac{1}{2n^s} + \frac{1}{n^{s+1}} [rn/rn]_{\Theta_s} \left(-\frac{1}{n^2} \right) + \sigma_{r,s,n}, \quad (21)$$

where

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

If $s < 0, s \notin \mathbb{Z}_{\leq 0}$, the degree of the numerator of the Padé must be increased, i.e. rn is replaced by $rn + p$ where $p = \lfloor -s/2 \rfloor + 1$. On the other hand, if s is not a real number, we could not prove that (21) still holds because $\nu_s(x)$ is no longer non-negative on its support. Consequently, the denominator of the Padé does not have its roots on $[0, +\infty)$, in which case our method is inoperant.

However, we can also use a similar approach as for Stieltjes' constants: we replace the Padé approximant in (21) by a Padé type approximant with a Wilson polynomial as generating polynomial. The following result is then obtained, the proof of which is not given here because it is very similar to that of Theorem 1.

We consider again the Wilson's polynomial $T_{rn}(\alpha, 1, x)$ as the generating polynomial for the Padé type approximants $(rn + p/rn)_{\Theta_s}$, with $\alpha := (m+5)/2 + p$ where m, n, p, r, s are specified below.

Theorem 3. *For any integers $n, p \geq 1$, any $r \in \mathbb{Q}_{\geq 0}$ such that $rn \in \mathbb{N}$, for any complex number s such that $\Re(s) > 0, s \neq 1$ and any integer $m > \Re(s) - 1$, we have*

$$\zeta(s) = \sum_{k=1}^n \frac{1}{k^s} + \frac{1}{(s-1)n^{s-1}} - \frac{1}{2n^s} + \frac{1}{n^{s+1}} (rn + p/rn)_{\Theta_s} \left(-1/n^2 \right) + \delta_{rn,p} \quad (22)$$

where

$$\limsup_{n \rightarrow \infty, rn \in \mathbb{N}} |\delta_{rn,p}|^{1/n} \leq \frac{(2r - \mu_r)^{2r}}{(2r + \mu_r)^{2r}} (1 - \mu_r) < 1$$

with $\mu_r = \frac{2r}{r + \sqrt{1+r^2}}$.

More precisely, we have

$$(rn + p/rn)_{\Theta_s}(z) = \sum_{j=0}^p c_j z^j + z^p \frac{N}{D}$$

where $m > \Re(s) - 1$, $\alpha = (m + 5)/2 + p$, $c_k := (-1)^k \frac{B_{2k+2}}{(2k+2)!}(s)_{2k+1}$,

$$N := \sum_{j=0}^{2rn} \frac{\binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1}}{j! \binom{\alpha+j}{j+1}} \sum_{q=0}^{j/2} \sum_{t=0}^{q-1} (-1)^q S(j+1, 2q+1) c_{t+p+1} \left(-\frac{1}{n^2}\right)^{t+1-q},$$

$$D := \sum_{j=0}^{2rn} \binom{2rn+1}{j+1} \binom{2rn+2\alpha+j}{j+1} \binom{n-1}{j} / \binom{\alpha+j}{j+1}.$$

Remark. If $s \in \mathbb{C}$, $s \notin \mathbb{Z}_{\leq 0}$, in Theorem 3 the degree of the Padé type approximant must be increased: p must be greater than $\lfloor -\Re(s/2) \rfloor + 1$, $m = 0$ and $\alpha = 5/2$. Hence, for every complex number $s \neq 1$, not in \mathbb{Z}^- , the convergence of formula (3) holds, with the same speed which is independent of p .

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