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▶ To cite this version:

Marc Prévost, Tanguy Rivoal. Application of Padé approximation to Euler's constant and Stirling's formula. 2019. hal-02017852v2

HAL Id: hal-02017852 https://hal.science/hal-02017852v2

Preprint submitted on 16 Mar 2019 (v2), last revised 9 Aug 2019 (v3)

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APPLICATION OF PADÉ APPROXIMATION TO EULER'S CONSTANT AND STIRLING'S FORMULA

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ABSTRACT. The Digamma function Γ'/Γ admits a well-known (divergent) asymptotic expansion involving Bernoulli's numbers. Using Touchard type orthogonal polynomials, we determine an effective bound for the error made when this asymptotic series is replaced by its nearly diagonal Padé approximants. By specialization, we obtain new fast converging sequences of approximations to Euler's constant γ . Even though these approximations are not strong enough to prove the putative irrationality of γ , we explain why they can be viewed, in some sense, as analogues of Apéry's celebrated sequences of approximations to $\zeta(2)$ and $\zeta(3)$. Similar ideas applied to the asymptotic expansion $\log \Gamma$ enable us to obtain a refined version of Stirling's formula.

1. Introduction

The Digamma function $\Psi(z) := \Gamma'(z)/\Gamma(z)$ is represented for any $z \in \mathbb{C} \setminus \mathbb{Z}_{\leq 0}$ by the convergent series

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

Here, γ denotes Euler's constant, classically defined as

$$\gamma := \lim_{k \to +\infty} \left(H_k - \log(k) \right)$$

where $H_k := \sum_{j=1}^k \frac{1}{j}$. In particular, $\Psi(1) = -\gamma$ and more generally, for any integer $n \ge 0$, $\Psi(n+1) = H_n - \gamma$, as follows from the functional equation

$$\Psi(n+z) = \Psi(z) + \sum_{k=0}^{n-1} \frac{1}{k+z}, \quad n \ge 0.$$

The (even) Bernoulli numbers $(B_{2n})_{n\geq 1}$ are defined by the power series expansion

$$\frac{t}{e^t - 1} + \frac{t}{2} - 1 = \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} t^{2n},\tag{1}$$

Date: March 16, 2019.

²⁰¹⁰ Mathematics Subject Classification. Primary 11Y60, 41A21; Secondary 11J72, 41A60.

Key words and phrases. Euler's constant, Gamma function, Digamma function, Stirling's formula, Bernoulli numbers, Padé approximants, Orthogonal polynomials.

which converges for $|t| < 2\pi$. It is well-known (see Section 2) that Ψ admits the expansion

$$\Psi(z) \sim \log(z) - \frac{1}{2z} - \sum_{n=1}^{\infty} \frac{B_{2n}}{2n} \cdot \frac{1}{z^{2n}}, \qquad z \in \mathbb{R}, z \to +\infty,$$
 (2)

where the series is divergent but asymptotic in the Poincaré sense.

Our first result is that (nearly) diagonal Padé approximants to the divergent series in (2) provide sequences of fast convergent approximations to Ψ . These sequences can be viewed as a way to sum the asymptotic expansion (2), and they fit into the Remainder Padé Approximants method introduced in [8]. As a special case, we obtain completely new sequences that converge quickly to γ .

We introduce the formal power series

$$\Phi(z) := \sum_{n=0}^{\infty} (-1)^n \frac{B_{2n+2}}{2n+2} z^n \in \mathbb{Q}[[z]].$$
 (3)

The basic properties of Padé approximation are recalled in §3, and below $[k-1/k]_{\Phi}(z) \in \mathbb{Q}(z)$ denotes the Padé approximant of Φ with numerator and denominator of degree $\leq k-1$ and $\leq k$ respectively.

Theorem 1. For any real number x > 0 and any integers $k \ge 1, n \ge 0$, we have

$$\Psi(x) = \log(x_n) - \sum_{j=0}^{n} \frac{1}{j+x} + \frac{1}{2x_n} - \frac{1}{x_n^2} \left[k - 1/k \right]_{\Phi} \left(-\frac{1}{x_n^2} \right) + \varepsilon_k(x_n) \tag{4}$$

where $x_n := x + n$ and

$$|\varepsilon_k(x_n)| \le \frac{(2k+1)(2k+2)}{(4k+3)x_n^{4k+2}} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}.$$
 (5)

When n is fixed, the right-hand side of (5) does not tend to 0 as $k \to +\infty$, and it is not clear whether $\varepsilon_k(x_n)$ tends to 0 or not in these conditions. On the other hand, when k is fixed and $n \to +\infty$, then $\varepsilon_k(x_n)$ tends to 0, but not very fast. In fact, a much faster convergence holds by letting k depend on n. For instance, we have the following corollary.

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

$$\gamma = H_n - \log(n) - \frac{1}{2n} + \frac{1}{n^2} \left[rn - 1/rn \right]_{\Phi} \left(-\frac{1}{n^2} \right) + \delta_{r,n}$$
 (6)

where $\delta_{r,n}$ is such that

$$\lim_{n \to +\infty, rn \in \mathbb{N}} \left| \delta_{r,n} \right|^{1/n} \le \left(\frac{r}{2e} \right)^{4r}. \tag{7}$$

To prove this corollary, we take in (4) x=1, change n to n-1, set k=rn and $\delta_{r,n}:=\varepsilon_{rn}(n)$. We obtain (6). Then, we apply Stirling's formula

$$n! = n^n e^{-n} \sqrt{2\pi n} (1 + o(1)), \qquad n \to +\infty$$
 (8)

to the righ-hand side of (5), and (7) follows. The sequence

$$g_{r,n} := H_n - \log(n) - \frac{1}{2n} + \frac{1}{n^2} \left[rn - 1/rn \right]_{\Phi} \left(-\frac{1}{n^2} \right)$$
 (9)

converges to γ at geometric speed as $n \to +\infty$, such that $rn \in \mathbb{N}$, and we explain in §7 why the sequences $(g_{r,n})_{n\geq 1}$ are, in some sense, analogues of Apéry's celebrated sequences of approximations to $\zeta(2)$ and $\zeta(3)$. Because of the term $\log(n)$ in $g_{r,n}$, the putative irrationality of γ cannot be deduced from the convergence of $g_{r,n}$ to γ by the usual irrationality criterions, simply because $g_{r,n} \notin \mathbb{Q}$. But such a deduction is also ruled out by the denominator d_n of the rational numbers $H_n - \frac{1}{2n} + \frac{1}{n^2} \left[rn - 1/rn \right]_{\Phi} \left(-\frac{1}{n^2} \right)$, which is numerically such that $d_n(\gamma - g_{r,n}) \to +\infty$.

Theorem 1 is very flexible. Indeed, every choice of k as a sub-linear function of n leads to a new sequence of approximations of values of $\Psi(x)$, though apparently not strong enough to prove an irrationality result when $x \in \mathbb{Q}$. In that case, Gauss' formula [6, p. 37, Eq. (5)] provides an expression of $\Psi(x)$ in terms of γ and logarithms of algebraic numbers, for instance $\Psi(1/2) = -\gamma - \log(4)$. A result similar to Corollary 1 could be stated for these values. For other sequences of rational approximations to γ built with Padé approximants for very different functions, we refer to [3, 12].

We now come to our second result. As recalled in §2, we have the well-known expansion

$$\log \left(\Gamma(z)\right) \sim z \log(z) - z$$

$$+ \frac{1}{2} \log(2\pi/z) + \sum_{n=1}^{\infty} \frac{B_{2n}}{2n(2n-1)} \cdot \frac{1}{z^{2n-1}}, \qquad z \to +\infty, z \in \mathbb{R}. \tag{10}$$

The series is divergent but asymptotic in Poincaré sense. Truncation of the series to the "smallest term" provides a refined version of Stirling's formula (8), i.e. an explicit form of the error term o(1). Other refined versions exist, where for instance the divergent series is replaced by certain convergent integrals (see Eqs. (18) and (19) in §2). We shall obtain a different refined version of Stirling's formula (8), based on the Padé approximants of the formal series

$$\Omega(z) := \sum_{n=0}^{\infty} (-1)^{n+1} \frac{B_{2n+4}}{(2n+4)(2n+3)} z^n \in \mathbb{Q}[[z]].$$
 (11)

We first state a result very similar to Theorem 1.

Theorem 2. For any real number x > 0 and any integers $k \ge 1, n \ge 0$, we have

$$\log (\Gamma(x_n)) = x_n \log(x_n) - x_n + \frac{1}{2} \log(2\pi/x_n) + \frac{1}{12x_n} - \frac{1}{x_n^3} [k - 1/k]_{\Omega} (-\frac{1}{x_n^2}) + \widehat{\varepsilon}_k(x_n)$$

where $x_n := x + n$ and

$$|\widehat{\varepsilon}_k(x_n)| \le \frac{(2k+1)(2k+2)}{(4k+3)x_n^{4k+2}} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}.$$

In particular, with x=1, n changed to n-1, k set equal to rn and $\widehat{\delta}_{r,n}:=\widehat{\varepsilon}_{rn}(n)$, we obtain the following refined version of Stirling's formula (8). Note that we need (8) to bound $(2rn)!^2/\binom{4rn+2}{2rn+1}^2$ and to derive (13), but the argument is not circular.

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

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

where

$$\limsup_{n \to +\infty} \left| \widehat{\delta}_{r,n} \right|^{1/n} \le \left(\frac{r}{2e} \right)^{4r}. \tag{13}$$

We did not try to compare the efficiency of (12) with respect to other existing algorithms to compute large values of n!; we simply view this result as another interesting application of our method.

The paper is organized as follows. The four following sections are devoted to the proofs of the theorems. In §2, we list many important formulas for $\Psi(z)$ and $\log(\Gamma(z))$. In §3, we recall various properties of Padé approximants. In §4 and §5, we give the proofs of Theorems 1 and 2; the main difficulty is in proving the convergence of the Padé approximants because no explicit expressions are known for their remainders in these precise situations. The last three sections are devoted to relevant comments on our results. In §6, we explain how to deduce from Corollary 1 fast converging sequences of rational approximations to γ free of any logarithm. We compare our results with those of Apéry in §7. Finally, in §8, we present some computations around Corollary 1 as well as a few open problems.

2. Formulas for $\Psi(z)$, $\log(\Gamma(z))$ and the Bernoulli numbers

In this section, we explain how the asymptotic expansions (2) and (10) can be obtained, and we also present two important integral representations of the Bernoulli numbers needed for the proofs of both theorems. We will first consider $\Psi(z)$ and then $\log(\Gamma(z))$. This material is classical and we don't claim any originality; it is important to recall it though.

We define $\log(z)$ for $z \in \mathcal{D} = \mathbb{C} \setminus (-\infty, 0]$ with its principal determination (i.e., $-\pi < \arg(z) < \pi$). The Digamma function admits various integral representations, in particular the following ones (attributed to Binet and Poisson respectively in [6, p. 201]):

$$\Psi(z) = \log(z) - \frac{1}{2z} - \int_0^\infty \left(\frac{1}{e^t - 1} + \frac{1}{2} - \frac{1}{t}\right) e^{-zt}, \quad \Re(z) > 0$$
 (14)

and

$$\Psi(z) = \log(z) - \frac{1}{2z} - \int_0^\infty \frac{2t}{(t^2 + z^2)(e^{2\pi t} - 1)} dt, \quad z \in \mathcal{D} \setminus i\mathbb{R}$$
 (15)

From the definition (1) of the Bernoulli numbers, we see that we can apply Watson's lemma [7, Chapter 2, §2] to the integral on the right-hand side of (14), and it follows that

 Ψ admits the expansion

$$\Psi(z) \sim \log(z) - \frac{1}{2z} - \sum_{n=1}^{\infty} \frac{B_{2n}}{2n} \cdot \frac{1}{z^{2n}}, \quad z \in \mathbb{R}, z \to +\infty$$

as expected.

We shall now prove that $((-1)^k \frac{B_{2k+2}}{2k+2})_{k\geq 0}$ is the moments sequence for the positive weight $\alpha(u) := \frac{1}{e^{2\pi\sqrt{u}}-1} \mathbf{1}_{[0,+\infty)}(u)$, where $\mathbf{1}_A$ denotes the indicator function of a set A. See also [6, p. 201, Eq. (48)].

Proposition 1. For every integer $k \geq 0$, we have

$$(-1)^k \frac{B_{2k+2}}{2k+2} = \int_0^\infty \frac{u^k}{e^{2\pi\sqrt{u}} - 1} du. \tag{16}$$

Proof. For any integer $N \geq 0$, we have

$$\frac{t^{2N} + (-1)^{N+1}z^{2N}}{t^2 + z^2} = \sum_{k=0}^{N-1} (-1)^{N-k-1}t^{2k}z^{2N-2k-2},$$

so that

$$\int_0^\infty \frac{2t}{(t^2 + z^2)(e^{2\pi t} - 1)} dt$$

$$= \sum_{k=0}^{N-1} \frac{(-1)^k}{z^{2k+2}} \int_0^\infty \frac{2t^{2k+1}}{e^{2\pi t} - 1} dt + \frac{(-1)^N}{z^{2N}} \int_0^\infty \frac{2t^{2N+1}}{(t^2 + z^2)(e^{2\pi t} - 1)} dt.$$

Hence for $z \in \mathcal{D} \setminus i\mathbb{R}$.

$$\Psi(z) = \log(z) - \frac{1}{2z} + \sum_{k=0}^{N-1} \frac{(-1)^{k+1}}{z^{2k+2}} \int_0^\infty \frac{2t^{2k+1}}{e^{2\pi t} - 1} dt + \frac{(-1)^{N+1}}{z^{2N}} \int_0^\infty \frac{2t^{2N+1}}{(t^2 + z^2)(e^{2\pi t} - 1)} dt.$$
 (17)

Eq. (17) is a finite form of the asymptotic expansion (2), because the integral is obviously $\mathcal{O}(1/z^2)$ as $z \to +\infty$. By unicity of such an expansion, it follows that for any integer $k \geq 0$,

$$(-1)^k \frac{B_{2k+2}}{2k+2} = \int_0^\infty \frac{2t^{2k+1}}{e^{2\pi t} - 1} dt = \int_0^\infty \frac{u^k}{e^{2\pi \sqrt{u}} - 1} du,$$

after the change of variable $t = \sqrt{u}$.

We now deal with various formulas for $\log (\Gamma(z))$. Integrating Binet's formula (14) between 0 and z, we get, for any z such that $\Re(z) > 0$

$$\log(\Gamma(z)) = z\log(z) - z + \frac{1}{2}\log(2\pi/z) + \int_0^\infty \frac{1}{t} \left(\frac{1}{e^t - 1} + \frac{1}{2} - \frac{1}{t}\right) e^{-zt} dt.$$
 (18)

The integration constant $\frac{1}{2}\log(2\pi)$ is a consequence of Stirling's formula (8), because the integral is o(1). Applying Watson's lemma to this integral, we obtain that

$$\log (\Gamma(z)) \sim z \log(z) - z + \frac{1}{2} \log(2\pi/z) + \sum_{n=1}^{\infty} \frac{B_{2n}}{2n(2n-1)} \cdot \frac{1}{z^{2n-1}}, \quad z \in \mathbb{R}, z \to +\infty,$$

as announced in the Introduction. Moreover, integrating Poisson's formula (15) between 0 and z, we get, for any $z \in \mathcal{D} \setminus i\mathbb{R}$:

$$\log (\Gamma(z)) = z \log(z) - z + \frac{1}{2} \log(2\pi/z) - 2 \int_0^\infty \frac{\arctan(z/t)}{e^{2\pi t} - 1} dt$$
$$= z \log(z) - z + \frac{1}{2} \log(2\pi/z) - \frac{z}{\pi} \int_0^\infty \frac{\log(1 - e^{-2\pi t})}{t^2 + z^2} dt.$$
(19)

The integration constant $\frac{1}{2}\log(2\pi)$ is again a consequence of (8), because the integral

is o(1). The second integral is obtained from the first one by integration by parts. We shall now prove that the sequence $((-1)^{k+1} \frac{B_{2k+4}}{(2k+3)(2k+4)})_{k \geq 0}$ is the moments sequence of the positive weight $\beta(u) := -\sqrt{u} \log(1 - e^{-2\pi\sqrt{u}})/(2\pi) \mathbf{1}_{[0,+\infty)}(u) \in L^1(\mathbb{R})$.

Proposition 2. For every integer $k \geq 0$, we have

$$(-1)^{k+1} \frac{B_{2k+4}}{(2k+3)(2k+4)} = -\frac{1}{2\pi} \int_0^\infty u^{k+1/2} \log(1 - e^{-2\pi\sqrt{u}}) du.$$
 (20)

Proof. Integrating by parts the equation (obtained in the proof of Proposition 1)

$$(-1)^k \frac{B_{2k+2}}{2k+2} = \int_0^\infty \frac{2t^{2k+1}}{e^{2\pi t}-1} dt, \quad \forall k \ge 0,$$

and changing k to k+1, we obtain, for any $k \geq 0$,

$$(-1)^{k+1} \frac{B_{2k+4}}{(2k+3)(2k+4)} = -\frac{1}{\pi} \int_0^\infty t^{2k+2} \log(1 - e^{-2\pi t}) dt$$

and (20) follows from the change of variable $t = \sqrt{u}$.

We deduce from (19) and the change of variable $t = \sqrt{u}$ that, for any $z \in \mathcal{D} \setminus i\mathbb{R}$,

$$\log(\Gamma(z)) = z\log(z) - z + \frac{1}{2}\log(2\pi/z) + \frac{B_2}{2z} - \frac{1}{z}\int_0^\infty \frac{\beta(u)}{z^2 + u}du.$$
 (21)

Note that (20) also holds for k=-1 which means that $((-1)^k \frac{B_{2k+2}}{(2k+1)(2k+2)})_{k\geq 0}$ is the moments sequence of the positive weight $\beta(u)/u \in L^1(\mathbb{R})$ but this property is not sufficient for our purpose.

3. Reminder of Padé approximants

In this section, we recall a few classical properties of Padé approximation theory.

Let $F(z) = \sum_{k=0}^{\infty} c_k z^k \in \mathbb{K}[[z]]$, where \mathbb{K} is a subfield of \mathbb{C} . For every given integers $p, q \geq 0$, there exist P(z) and $Q(z) \in \mathbb{K}[z]$, $Q \neq 0$, and of respective degrees $\leq p$ and $\leq q$, such that $z^{-p-q-1}(Q(z)F(z)-P(z)) \in \mathbb{C}[[z]]$. The existence of $Q \neq 0$ is immediate because it amounts to the resolution of a non-trivial system of q linear equations (the vanishing conditions) with q+1 indeterminates (the coefficients of Q), and P is then uniquely associated to Q. The (reduced) rational fraction P/Q is unique and is by definition the Padé approximant $[p/q]_F$ of F.

We have the general expression

$$Q(z) = \eta_{p,q} \begin{vmatrix} c_{p-q+1} & c_{p-q+2} & \cdots & c_{p+1} \\ \vdots & \vdots & \cdots & \vdots \\ c_p & c_{p+1} & \cdots & c_{p+q} \\ z^q & z^{q-1} & \cdots & 1 \end{vmatrix}$$
(22)

where $\eta_{p,q} \in \mathbb{K}^*$ is arbitrary, and by convention $c_k = 0$ if $k \leq -1$. There also exists a (more complicated) determinantal expression for P(z), but we can also use $P(z) = [Q(z)F(z)]_{\leq p}$, the truncation of the Taylor expansion of Q(z)F(z) up to z^p . From (22), we see that Q(z) has degree exactly q if, and only if, the Hankel determinant

$$H_q(c_{p-q+2}) := \begin{vmatrix} c_{p-q+2} & c_{p-q+3} & \cdots & c_{p+1} \\ c_{p-q+3} & c_{p-q+4} & \cdots & c_{p+2} \\ \vdots & \vdots & \ddots & \vdots \\ c_{p+1} & c_{p+2} & \cdots & c_{p+q} \end{vmatrix} \neq 0.$$

Moreover, $Q(0) \neq 0$ if, and only if, the Hankel determinant

$$H_q(c_{p-q+1}) := \begin{vmatrix} c_{p-q+1} & c_{p-q+2} & \cdots & c_p \\ c_{p-q+2} & c_{p-q+3} & \cdots & c_{p+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_p & c_{p+1} & \cdots & c_{p+q-1} \end{vmatrix} \neq 0.$$

Of particular interest to us is the case of $F(z) = \int_{\mathbb{R}} \frac{\omega(u)}{1-uz} du$ where $\omega \in L^1(\mathbb{R})$ is such that $\omega(u) \geq 0$ for all $u \in \mathbb{R}$, and the support of ω , say S, is a closed subinterval of \mathbb{R} . The function F is analytic (at least) at any z such that $1/z \notin S$. We further assume that

$$0 < m_k := \int_{\mathbb{R}} u^k \omega(u) du < \infty, \quad \forall k \ge 0.$$

Then, for all $N \geq 0$,

$$F(z) = \sum_{k=0}^{N-1} m_k z^k + z^N \int_{\mathbb{R}} \frac{u^N}{1 - uz} \omega(u) du,$$

so that m_k is the k-th Taylor coefficient of F at z=0. It follows that the function F is also C^{∞} at z=0, and formally $F(z)=\sum_{k=0}^{\infty}m_kz^k$. Consider a sequence $(q_k)_{k\geq 0}$ of orthogonal polynomials with respect to ω , i.e.

$$\int_{\mathbb{R}} u^j q_k(u)\omega(u)du = 0, \quad \forall j, k, \ 0 \le j < k$$

with $q_0(z) := 1$; each q_k is of degree k, see below. For any $k \ge 0$, we set

$$p_k(z) := \int_{\mathbb{R}} \frac{q_k(z) - q_k(u)}{z - u} \omega(u) du,$$

which is a polynomial of degree $\leq k-1$ (equal to 0 if k=0), and we also set

$$R_k(z) := z^k \int_{\mathbb{R}} \frac{q_k(u)}{1 - zu} \omega(u) du.$$

For simplicity, let $Q_k(z) := z^k q_k(1/z)$ and $P_k(z) := z^{k-1} p_k(1/z)$. A straightforward computation shows that

$$R_k(z) = Q_k(z)F(z) - P_k(z).$$

Moreover, since $\frac{1-(zu)^k}{1-zu}$ is a polynomial in u of degree k-1, we have by orthogonality

$$R_k(z) = z^k \underbrace{\int_{\mathbb{R}} \frac{1 - (zu)^k}{1 - zu} q_k(u)\omega(u) du}_{= 0} + z^{2k} \int_{\mathbb{R}} \frac{u^k q_k(u)}{1 - zu} \omega(u) du.$$

Hence, $R_k(z) \in z^{2k}\mathbb{C}[[z]]$, which means in other words that (1)

$$\frac{P_k(z)}{Q_k(z)} = [k - 1/k]_F(z).$$

In that case, both $H_q(m_{p-q+1}) = H_k(m_0)$ and $H_q(m_{p-q+2}) = H_k(m_1)$ (with p = k-1 and q = k) are automatically non-zero for any $p, q \ge 0$ (by [5, p. 116, Eq. (2.48)]), so that for any $k \ge 0$, Q_k is of degree k and $Q_k(0) \ne 0$ (or, equivalently, q_k is of degree k and $q_k(0) \ne 0$). Moreover, the zeros of $q_k(z)$ are located on the support S of ω .

Proposition 3. For any $z \in \mathbb{C}$ such that $1/z \notin S$ and any integer $k \geq 1$, we have

$$F(z) - [k - 1/k]_F(z) = \frac{1}{q_k(1/z)^2} \int_{\mathbb{D}} \frac{q_k(u)^2}{1 - zu} \omega(u) du = \frac{z^{2k}}{Q_k(z)^2} \int_{\mathbb{D}} \frac{q_k(u)^2}{1 - zu} \omega(u) du.$$
 (23)

Proof. Note that $\frac{q_k(u)-q_k(1/z)}{1-zu}$ is a polynomial in u of degree $\leq k-1$. Hence by orthogonality, we have

$$\int_{\mathbb{R}} \frac{q_k(u)^2}{1 - zu} \omega(u) du = \underbrace{\int_{\mathbb{R}} q_k(u) \frac{q_k(u) - q_k(1/z)}{1 - zu} \omega(u) du}_{= 0} + \underbrace{q_k(1/z) \int_{\mathbb{R}} \frac{q_k(u)}{1 - zu} \omega(u) du}_{= z^{-k} q_k(1/z) R_k(z)}.$$

¹We make here a slight abuse of notation, i.e. $[k-1/k]_F(z)$ should be noted $[k-1/k]_{\widehat{F}}(z)$, where $\widehat{F}(z) := \sum_{k=0}^{\infty} m_k z^k \in \mathbb{K}[[z]]$.

This is (23) in a different form.

A similar argument shows that, more generally, for any integers m, n such that $m \ge n - 1 \ge 0$, and any $z \in \mathbb{C}$ such $1/z \notin S$, we have

$$F(z) - [m/n]_F(z) = \frac{z^{m-n+1}}{q_n(1/z)^2} \int_{\mathbb{R}} u^{m-n+1} \frac{q_n(u)^2}{1 - zu} \omega(u) du.$$

As we shall see, Eq. (23) is important because of the following proposition. For j = 1 or j = 2, we denote by $(q_{j,k})_{k\geq 0}$ the sequence of orthogonal polynomials with respect to a positive weight ω_j with the same properties as above.

Proposition 4. Assume that for any $u \in \mathbb{R}$, we have $0 \le \omega_1(u) \le \omega_2(u)$, and that each $q_{j,k}$ is unitary. Then for every integer $k \ge 0$, we have

$$\int_{\mathbb{R}} q_{1,k}(u)^2 \omega_1(u) du \le \int_{\mathbb{R}} q_{2,k}(u)^2 \omega_2(u) du.$$

Proof. We shall use the following fact (see [5, p. 60]). In the above conditions, let q_k denotes the orthogonal polynomial of degree k with respect to $\omega \geq 0$, and assumed to be unitary. Then q_k realizes the minimum for the norm in $L^2(\mathbb{R})$ of the \mathbb{R} -linear form $p \mapsto \int_{\mathbb{R}} p(u)\omega(u)du$ amongst all unitary polynomials $p(X) \in \mathbb{R}[X]$ of degree k.

Indeed, for such a polynomial p, there exist k real numbers $\alpha_0, \alpha_1, \dots, \alpha_{k-1}$ such that

$$p(u) = \sum_{j=0}^{k} \alpha_j q_j(u)$$

where $\alpha_k := 1$. Then

$$\int_{\mathbb{R}} p(u)^{2} \omega(u) du = \sum_{i=0}^{k} \sum_{j=0}^{k} \alpha_{i} \alpha_{j} \int_{\mathbb{R}} q_{i}(u) q_{j}(u) \omega(u) du$$

$$= \sum_{j=0}^{k} \alpha_{j}^{2} \int_{\mathbb{R}} q_{j}(u)^{2} \omega(u) du \qquad \text{(orthogonality)}$$

$$\geq \int_{\mathbb{R}} q_{k}(u)^{2} \omega(u) du \qquad (\alpha_{k} = 1).$$

Now, coming back to the notations of the proposition, since $\omega_1 \leq \omega_2$, we get for any k > 0 that

$$\int_{\mathbb{R}} q_{1,k}(u)^2 \omega_1(u) du \leq \int_{\mathbb{R}} q_{2,k}(u)^2 \omega_1(u) du \qquad \text{(minimisation of the linear form)}$$

$$\leq \int_{\mathbb{R}} q_{2,k}(u)^2 \omega_2(u) du \qquad (\omega_1 \leq \omega_2).$$

This completes the proof of the proposition.

4. Proof of Theorem 1

We shall use the following results. For every $k \geq 0$, let

$$W_k(z) = \sum_{j=0}^k {k+1 \choose j+1} {k+j+2 \choose j+1} {z-1 \choose j},$$

which is a polynomial of degree k and of the same parity as k. The sequence $(W_k(z))_{k\geq 0}$ satisfies the orthogonality relations

$$\int_{i\mathbb{R}} W_m(x)W_n(x) \frac{\pi x^2}{\sin^2(\pi x)} dx = \begin{cases} 0 & \text{if } m \neq n \\ (-1)^m \frac{2i(m+1)(m+2)}{2m+3} & \text{if } m = n. \end{cases}$$
(24)

See [4, p. 653, Eqs. (2.10) and (2.13)] with the parameters α and γ set to 1, as well as [8, 13] for further properties.

We now let $\delta(u) := \frac{2\pi\sqrt{u}e^{2\pi\sqrt{u}}}{(e^{2\pi\sqrt{u}}-1)^2}\mathbf{1}_{[0,+\infty)}(u) \in L^1(\mathbb{R})$. The sequence of unitary orthogonal polynomials $(T_k(z))_{k\geq 0}$ on $[0,+\infty)$ with respect to α are thus given by

$$T_k(z) = \frac{(2k)!}{\binom{4k+2}{2k+1}} W_{2k}(i\sqrt{z}).$$

In particular, Eq. (24) becomes

$$\int_0^\infty T_k^2(u)\delta(u)du = \frac{(2k+1)(2k+2)}{4k+3} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}, \qquad \forall k \ge 0.$$
 (25)

We recall that $\alpha(u) := \frac{1}{e^{2\pi\sqrt{u}}-1} \mathbf{1}_{[0,+\infty)}(u) \in L^1(\mathbb{R})$. Note that the Taylor expansion at t=0 of $\int_0^\infty \frac{\alpha(u)}{1-tu} du$ is $\Phi(t)$ by Proposition 1. Let $q_k(z)$ be the kth unitary orthogonal polynomial on $[0,+\infty)$ with respect to α . We also let $Q_k(z) := z^k q_k(1/z)$. Contrary to the weight $\delta(u)$, no explicit expression for the polynomials q_k is known, beyond the general formula

$$q_k(z) = \frac{(-1)^{k+1}}{H_k(b_1)} \begin{vmatrix} b_0 & b_1 & \cdots & b_k \\ \vdots & \vdots & \cdots & \vdots \\ b_{k-1} & b_k & \cdots & b_{2k-1} \\ z^k & z^{k-1} & \cdots & 1 \end{vmatrix}$$

given by (22) with p = k - 1, q = k and $b_j := (-1)^j \frac{B_{2j+2}}{2j+2}$. However, we will be able to use the polynomials T_k in this case as well. Since the zeros of the unitary polynomial q_k are in $[0, +\infty)$, it follows that for any real number t < 0, we have $|q_k(t)| \ge |t|^k$.

A simple but crucial observation is that $\alpha(u) \leq \delta(u)$ for every $u \geq 0$ because $e^u \geq u + 1$ for every $u \geq 0$. Let now t be a fixed negative real number. From the various properties

collected in Section 3 and above, we have

$$\begin{split} \frac{1}{q_k(1/t)^2} \int_0^\infty \frac{q_k^2(u)}{1-tu} \alpha(u) du &\leq \frac{1}{q_k(1/t)^2} \int_0^\infty q_k^2(u) \alpha(u) du \\ &\leq t^{2k} \int_0^\infty q_k^2(u) \alpha(u) du \\ &\leq t^{2k} \int_0^\infty T_k^2(u) \alpha(u) du \\ &\leq t^{2k} \int_0^\infty T_k^2(u) \delta(u) du \\ &= t^{2k} \frac{(2k+1)(2k+2)}{4k+3} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}. \end{split}$$

By Proposition 3, it follows that, for every t < 0,

$$\left| \int_0^\infty \frac{\alpha(u)}{1 - tu} du - \left[k - 1/k \right]_{\Phi}(t) \right| \le t^{2k} \frac{(2k+1)(2k+2)}{4k+3} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}.$$

From (15), we have

$$\Psi(z) = \log(z) - \frac{1}{2z} - \frac{1}{z^2} \int_0^\infty \frac{\alpha(u)}{1 + u/z^2} du, \quad z \in \mathcal{D} \setminus i\mathbb{R}.$$

Therefore, for any real number x > 0 and any integers $k \ge 1, n \ge 0$, we have

$$\Psi(x_n) = \log(x_n) - \frac{1}{2x_n} - \frac{1}{x_n^2} \left[k - 1/k \right]_{\Phi} \left(-\frac{1}{x_n^2} \right) + \varepsilon_k(x_n)$$

with $x_n := x + n$ and

$$|\varepsilon_k(x_n)| \le \frac{(2k+1)(2k+2)}{(4k+3)x_n^{4k+2}} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}.$$

The identity

$$\Psi(x_n) = \Psi(x) + \sum_{k=0}^{n-1} \frac{1}{k+x}$$

completes the proof of the theorem.

5. Proof of Theorem 2

The proof is very similar to that of Theorem 1, so that we will skip most details. We recall that $\beta(u) := -\sqrt{u} \log(1 - e^{-2\pi\sqrt{u}})/(2\pi) \mathbf{1}_{[0,+\infty)}(u)$.

Straightforward computations shows that for any $u \geq 0$, we have

$$0 \le -\sqrt{u}\log(1 - e^{-2\pi\sqrt{u}}) \le \frac{\sqrt{u}}{e^{2\pi\sqrt{u}} - 1} \le \frac{\sqrt{u}e^{2\pi\sqrt{u}}}{(e^{2\pi\sqrt{u}} - 1)^2}.$$

It follows that $0 \leq \beta(u) \leq \delta(u)$ for any $u \in \mathbb{R}$, where $\delta(u) := \frac{2\pi\sqrt{u}e^{2\pi\sqrt{u}}}{(e^{2\pi\sqrt{u}}-1)^2}\mathbf{1}_{[0,+\infty)}(u)$ is the weight function used in §4.

We are thus exactly in the same situation as in §4 and by Proposition 3, for every t < 0 and any integer $k \ge 1$, we have

$$\left| \int_0^\infty \frac{\beta(u)}{1 - tu} du - \left[k - 1/k \right]_{\Omega}(t) \right| \le t^{2k} \frac{(2k+1)(2k+2)}{4k+3} \cdot \frac{(2k)!^2}{\binom{4k+2}{2k+1}^2}.$$

The conclusion of Theorem 2 follows from Eq. (21) in §2 and $B_2 = \frac{1}{6}$, using similar steps as those in the proof of Theorem 1.

6. Rational approximations to Euler's constant

Padé approximants can be computed fairly efficiently with the ε -algorithm (see [5, Chapter 3, §3.3]); the presence of $\log(n)$ in Corollary 1 is minor because it can also be computed efficiently. Nonetheless, we present in this section two different ways to obtain sequences of rational approximations to γ from Corollary 1. For simplicity, we set r=1 throughout this section.

In the first approach, we use (6) twice with $n=a^m$ and $n=a^{m+1}$ respectively, for some integers $a\geq 2$ and $m\geq 0$. Both logarithms can then be cancelled by the trivial equation $m\log(a^{m+1})-(m+1)\log(a^m)=0$, so that letting

$$\rho_m(a) := (m+1)H_{a^m} - mH_{a^{m+1}} - \frac{m+1}{2a^m} + \frac{m}{2a^{m+1}} + \frac{m+1}{a^{2m}} \left[a^m - 1/a^m \right]_{\Phi} (-a^{-2m}) - \frac{m}{a^{2m+2}} \left[a^{m+1} - 1/a^{m+1} \right]_{\Phi} (-a^{-2m-2}) \in \mathbb{Q},$$

we have

$$|\gamma - \rho_m(a)| \le (2e)^{-4 \cdot a^m (1 + o(1))}, \qquad m \to +\infty.$$
 (26)

The speed of convergence in (26) is fast. However, the sequence of denominators of $\rho_m(a)$ appears again to tend to ∞ much faster than $(2e)^{4\cdot a^m}$ and it seems that there is no choice of a for which we can deduce from (26) that $\gamma \notin \mathbb{Q}$.

In the second approach, we use (6) with $n=2^m$ for any $m\geq 0$. We do not cancel exactly $m\log(2)$ as above, but instead we replace $\log(2)$ by a suitable Padé approximant to $L(z):=\log(1-z)$ at z=-1 (see [9] for a similar idea). We recall the following well-known facts (see [1]). For any integer $n\geq 0$, let $P_n(z)=\frac{1}{n!}(z^n(1-z)^n)^{(n)}\in\mathbb{Z}[z]$ denotes the n-th Legendre polynomial and $Q_n(z)=\int_0^1\frac{P_n(u)-P_n(z)}{z-u}du\in\mathbb{Q}[z]$ of degree n-1. Then, for any $z\in\mathbb{C}$ such $|z|\leq 1$, $z\neq 1$, and any integer $n\geq 0$, we have

$$[n/n]_L(z) = \frac{z^n Q_n(1/z)}{z^n P_n(1/z)}$$

and

$$\kappa_n := \left| \log(2) - [n/n]_L(-1) \right| \le (\sqrt{2} - 1)^{4n + o(n)}, \quad n \to +\infty.$$
(27)

We now define

$$r_m := H_{2^m} - \frac{1}{2^{m+1}} - m[2^m/2^m]_L(-1) + \frac{1}{4^m}[2^m - 1/2^m]_{\Phi}(-4^{-m}) \in \mathbb{Q}.$$

Since, as $m \to +\infty$,

$$|\delta_{1,2^m}| + \kappa_{2^m} \le (2e)^{-2^{m+2}(1+o(1))} + (\sqrt{2}-1)^{2^{m+2}(1+o(1))},$$

Eqs. (6) and (27) imply that

$$|\gamma - r_m| \le (\sqrt{2} - 1)^{2^{m+2}(1+o(1))}, \quad m \to +\infty.$$

Again, it does not seem possible to deduce that $\gamma \notin \mathbb{Q}$ from this sequence of approximations.

7. Connection with Apéry's sequences

In [8], the first author gave a new method to constuct rational approximations to $\zeta(2)$ and $\zeta(3)$. Surprisingly, doing so, he recovered Apéry's sequences to these numbers and obtained another proof of their irrationality. We now give a quick overview of this construction, which is at the origin of the results of the present paper. This will explain the comment made in the Introduction that the sequence of approximations to γ in Corollary 1 are in some sense analoguous to Apéry's sequences.

For any integer $s \geq 2$, let

$$\Psi_s(z) = \Gamma(s) \sum_{k=1}^{\infty} \frac{1}{(k+z)^s} = \int_0^{\infty} u^{s-1} \frac{e^{-uz}}{e^u - 1} du.$$

The series converges for any $z \in \mathbb{C} \setminus \mathbb{Z}_{\leq -1}$, while the integral converges for $\Re(z) > -1$. Note that the function Digamma function $\Psi(z)$ is a convergent version of the divergent $\Psi_1(z-1)$. Let

$$\Phi_s(z) = \sum_{n=0}^{\infty} \frac{\Gamma(n+s-1)}{n!} B_n z^{n+s-1} \in \mathbb{Q}[[z]].$$

Note that $z^2\Phi(-z^2)$ is essentially equal (2) to $\Phi_1(z)$, provided the terms n=0 and n=1 are removed in the series for $\Phi_1(z)$. Then for any integer $s \geq 2$, the function $\Psi_s(z)$ admits $\Phi_s(1/z)$ as asymptotic expansion as $z \to +\infty$, $z \in \mathbb{R}$. For any integer $n \geq 0$, we have

$$\zeta(s) = \sum_{k=1}^{n} \frac{1}{k^s} + \frac{1}{\Gamma(s)} \Psi_s(n),$$

which are analogues of $\gamma = H_n - \Psi(n+1)$. It is then natural to consider the Padé approximants $[p/q]_{\Phi_s}(z)$ and to find out for which values of the integers $p, q \geq 0$, we have

$$\zeta(s) \approx \sum_{k=1}^{n} \frac{1}{k^s} + [p/q]_{\Phi_s} \left(\frac{1}{n}\right). \tag{28}$$

It seems difficult to solve this problem, but this was done for s=2 and s=3 in [8].

²The variable $-z^2$ instead of z explains why the Padé approximants in this paper are evaluated at $-\frac{1}{n^2}$ and not $\frac{1}{n}$ as in [8].

In the case s = 2, let us consider the sequence of Touchard polynomials [13]

$$\Omega_k(z) = \sum_{j=0}^k \binom{k}{j} \binom{k+j}{j} \binom{z}{j}, \quad k \ge 0$$

which are of degree k and very similar to the polynomials $W_k(z)$ introduced in §4; in particular the sequence $(\Omega_k(u))_{k\geq 0}$ is orthogonal for the weight $1/\sin^2(\pi u)$ for $u\in -\frac{1}{2}+i\mathbb{R}$. Then $z^n\Omega_n(1/z)$ is the denominator of $[n/n]_{\Phi_2}(z)$ and

$$\sum_{k=1}^{n} \frac{1}{k^2} + [n/n]_{\Phi_2} \left(\frac{1}{n}\right)$$

is related to the sequence of approximations to $\zeta(2)$ discovered by Apéry. More precisely, $\Omega_n(n) = \sum_{j=0}^n \binom{n}{j}^2 \binom{n+j}{j}$ and

$$\zeta(2) - \left(\sum_{k=1}^{n} \frac{1}{k^2} + [n/n]_{\Phi_2} \left(\frac{1}{n}\right)\right) = \Omega_n(n)^{-1} \left(\frac{\sqrt{5} - 1}{2}\right)^{5n + o(n)},$$

which shows that (28) holds for s=2 in a strong sense. See also [11] for another use of the polynomials $\Omega_k(z)$ to construct rational approximations to Catalan's constant $\sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}$.

In the case s = 3, let us consider the sequence of polynomials

$$\Pi_{2k}(z) = \sum_{j=0}^{k} {k \choose j} {k+j \choose j} {z+j \choose j} {z \choose j}, \quad k \ge 0.$$

They are related to Wilson polynomials [14] and are of degree 2k. The sequence $(\Pi_{2k}(iu - \frac{1}{2}))_{k\geq 0}$ is (essentially) orthogonal for the weight $u\sinh(\pi u)/\cosh^3(\pi u)$ for $u\in\mathbb{R}$. Then $z^{2n}\Pi_{2n}(1/z)$ is the denominator of $[2n/2n]_{\Phi_3}(z)$ and

$$\sum_{k=1}^{n} \frac{1}{k^3} + [2n/2n]_{\Phi_3} \left(\frac{1}{n}\right)$$

is now related to the sequence of approximations to $\zeta(3)$ discovered by Apéry. More precisely, $\Pi_{2n}(n) = \sum_{j=0}^{n} \binom{n}{j}^2 \binom{n+j}{j}^2$ and

$$\zeta(3) - \left(\sum_{k=1}^{n} \frac{1}{k^3} + [2n/2n]_{\Phi_3} \left(\frac{1}{n}\right)\right) = \Pi_{2n}(n)^{-1} \left(\sqrt{2} - 1\right)^{4n + o(n)},$$

which again shows that (28) holds for s = 3 in a strong sense.

Unfortunately, the pattern breaks down for $s \geq 4$ because no explicit sequences of orthogonal polynomials are known. However, the method presented in this paper (based on positivity of weights) might apply and we plan to elaborate on the subject in the future, using the weights representations given in [10].

8. Numerical computations

The first four Padé approximants $[k-1/k]_{\Phi}(z)$, k=1,2,3,4, of the formal series $\Phi(z)$ (defined in (3)) are

$$\frac{5}{6(10-z)}, \quad \frac{7(790-871z)}{20(241z^2-3990z+3318)}, \\ \frac{-39577260671z^2+66288226620z-15762446700}{1260(20169451z^3-434410620z^2+646328298z-150118540)}$$

and

$$\begin{aligned} &11\big(-66121532483928871z^3 + 154759983905137780z^2\\ &-68434474957415658z + 6638618337225420\big)\\ &/\big(2520\big(162262595834387z^4 - 4153727584332260z^3\\ &+8451860104365678z^2 - 3619436689059620z + 347737150997522\big)\big)\end{aligned}$$

The first four approximations $g_{1,n}$, n = 1, 2, 3, 4, to γ (defined in (9)) are

$$\frac{19}{33}, \frac{880221}{692890} - \log(2), \frac{349922562423851}{208805779764540} - \log(3), \frac{14082424058723999186111}{7172066285428422496860} - \log(4)$$
 and they are quickly convergent:

$$|\gamma - g_{1,1}| < 1.46 \cdot 10^{-3}, \qquad |\gamma - g_{1,2}| < 1.03 \cdot 10^{-6}$$

 $|\gamma - g_{1,3}| < 8.26 \cdot 10^{-10}, \qquad |\gamma - g_{1,4}| < 6.88 \cdot 10^{-13}.$

Numerically, it seems that

$$\lim_{n \to +\infty} |\gamma - g_{1,n}|^{1/n} \approx 0.00087,$$

which indicates that our bound (given by (7))

$$\limsup_{n \to +\infty} |\gamma - g_{1,n}|^{1/n} \le (2e)^{-4} \approx 0.00114$$

might not be too far off.

Let $(D_n)_{n\geq 1}$ denotes the sequence of denominators of $[n-1/n]_{\Phi}(-\frac{1}{n^2})$ (in reduced form). The first seven values of D_n are

66, 346445, 23200642196060, 1793016571357105624215,

15228279926117654663108958325260625655928,

192235689436727179266849483169227464609368863628487420075870,

18288050792990287112994873911376782419504189190149640569292355143723862909911720.

Numerical computations (made for $1 \le n \le 180$) suggest that there exists a constant $c \approx 1.71$ such that $\log(D_n) \sim cn^2 \log(n)$.

As seen in §7, the respective denominators of $[n/n]_{\Phi_2}(z)$ and $[2n/2n]_{\Phi_3}(z)$ are equal to $z^n\Omega_n(1/z)$ and $z^{2n}\Pi_{2n}(1/z)$, which both satisfy linear recurrences with coefficients in

 $\mathbb{Q}[n,z]$. Moreover, the denominators of the rational numbers $[n/n]_{\Phi_2}(\frac{1}{n})$ and $[2n/2n]_{\Phi_3}(\frac{1}{n})$ can then be expressed in terms of (but are not exactly equal to) the Apéry sequences $\Omega_n(n) = \sum_{j=0}^n {n \choose j}^2 {n+j \choose j}$ and $\Pi_{2n}(n) = \sum_{j=0}^n {n \choose j}^2 {n+j \choose j}^2$. Both satisfy a linear recurrence of order 2 with coefficients in $\mathbb{Q}[n]$, and their respective growth rates are $(\frac{\sqrt{5}+1}{2})^{5n+o(n)}$ and $(\sqrt{2}+1)^{4n+o(n)}$.

This suggests the following questions, where $Q_n(z)$ denotes the denominator of $[n-1/n]_{\Phi}(z)$, normalized to be unitary.

- (i) Does there exist a (multiple) hypergeometric sum formula for $Q_n(z)$, like for $\Omega_n(z)$ and $\Pi_{2n}(z)$?
- (ii) Does the sequence $(\mathcal{Q}_n(z))_{n\geq 1}$ satisfy a linear recurrence of finite order with coefficients in $\mathbb{Q}[n,z]$?
- (iii) Does the sequence $(\mathcal{Q}_n(-1/n^2))_{n\geq 1}$ satisfy a linear recurrence of finite order with coefficients in $\mathbb{Q}[n]$?
- (iv) Is it true that, as $n \to +\infty$, $\log(D_n) \sim cn^2 \log(n)$ for some constant c > 0?
- (v) Does the limit of $|\gamma g_{1,r}|^{1/n}$ exist as $n \to +\infty$?

Note that there is no obvious relation between D_n and $Q_n(-1/n^2)$ (which is not an integer) because the numerator of $[n-1/n]_{\Phi}(z)$ also contributes to D_n when it is evaluated at $z=-1/n^2$.

By the theory of orthogonal polynomials (see [5, p. 43, Theorem 2.4]), we know that the sequence $(Q_n(z))_{n\geq 1}$ satisfies a linear recurrence of order 2: its coefficients are polynomials in z (of degree 1) but they are not polynomials in n. A negative answer to (ii) would automatically provide a negative answer to (i).

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