

ON THE NUMERICAL CALCULATION OF EULER'S GAMMA CONSTANT *

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0. Historical background

Euler's constant

$$\gamma = \lim_{n \rightarrow +\infty} 1 + \frac{1}{2} + \cdots + \frac{1}{n} - \log n,$$

also called sometimes the Euler-Mascheroni constant, has been the subject of many studies and numerical evaluations since the eighteenth century. Nevertheless, it still retains much of its mystery today. For instance, it remains unclear whether or not γ is irrational, in spite of several attempts of proof. Let us mention e.g. that of P. Appell [2] in 1926, which failed due to a material error, and that of A. Froda [14] in 1965, that is based on a still incompletely proved criterion of irrationality. However, we should mention that some transcendence results for expressions involving γ have been obtained by K. Mahler [18].

Here we focus mainly on the description of some techniques that provide quickly convergent algorithms. Besides their computational interest, such algorithms might hopefully lead in the future to results of an arithmetic nature.

The first evaluation of γ is due naturally to Leonhard Euler, who obtained the value 0.577218 in 1735 [12], soon extended by Mascheroni and others. In 1781, Euler determined in [13] the more accurate value 0.577215664901532. It was followed by C.F. Gauss with a 22 decimal places value, and then by a number of English mathematicians of the nineteenth century. The reader is referred to J.W.L. Glaisher [15] for a detailed history of calculations made prior to 1870. In 1867-1871, W. Shanks [19] published 110 decimal places, of which 101 were accurate; soon afterwards, the famous mathematician-astronomer J.C. Adams [1] laboriously calculated 263 digits, a result that remained the world record since its publication in 1878 until the advent of the first computers and the 328 digit value obtained by J.W. Wrench Jr. [23] in 1952.

* This paper is an extended version of an original text written in June 1984 and published in "Gazette des Mathématiciens" in 1985. However, because of length constraints for the publication, the main idea for obtaining the error estimate of the Brent-McMillan algorithm had been only hinted, and most of the details had then been omitted. After more than 30 years passed, we take the opportunity to make these details finally available in the form of a \TeX manuscript.

All these calculations, as well as the subsequent one conducted by D.E. Knuth [17] in 1962 with 1 271 D, were based on the asymptotic expansion of $1 + \frac{1}{2} + \dots + \frac{1}{n} - \log n$ provided by the Euler-Maclaurin formula. The prohibitive time required by the calculation of Bernoulli numbers in this method led Dura W. Sweeney [21] to introduce a new more efficient algorithm, based on the formula $\gamma = -\int_0^{+\infty} \log x e^{-x} dx$. In this way, Sweeney obtained 3 566 D in 1963, and her method was also later adopted by Beyer-Waterman [3] [4] in 1974 (7 114 D, of which only 4 879 were correct) and by R.P. Brent [7], [8] (20 700 D in 1977). Finally in 1980, R.P. Brent and E. Mc Millan [10] discovered a new more efficient algorithm relying on a use of Bessel functions, and computed 30 100 D, see [9]. The goal of this brief overview is to present the above mentioned algorithms, along with a comparative analysis of the corresponding time complexity.

1. The Euler-Maclaurin formula

This classical formula will be used as follows (see e.g. Bourbaki [5]):

$$\sum_{i=1}^n f(i) = \int_1^n f(x) dx + \frac{1}{2}(f(n) + f(1)) + \sum_{j=1}^k \frac{b_{2j}}{(2j)!} \left[f^{(2j-1)}(n) - f^{(2j-1)}(1) \right] + R_k$$

where b_j is the sequence of Bernoulli numbers, defined by

$$\frac{z}{e^z - 1} = \sum_{j=0}^{+\infty} \frac{b_j}{j!} z^j,$$

so that

$$b_0 = 1, \quad b_1 = -\frac{1}{2}, \quad b_2 = \frac{1}{6}, \quad b_3 = 0, \quad b_4 = -\frac{1}{30}, \quad b_{2k+1} = 0, \quad \dots$$

The remainder term R_k is given by

$$R_k = \frac{1}{(2k+1)!} \int_1^n B_{2k+1}(\{x\}) f^{(2k+1)}(x) dx,$$

where $B_m(x) = \sum_{j=0}^m \binom{m}{j} b_j x^{m-j}$ is m -th Bernoulli polynomial and $\{x\}$ denotes the fractional part of x . If we take $f(x) = \frac{1}{x}$, the above formula becomes (see e.g. D. Knuth [17]):

$$\begin{aligned} & 1 + \frac{1}{2} + \dots + \frac{1}{n} \\ &= \log n + \frac{1}{2} + \frac{1}{2n} + \frac{b_2}{2} \left(1 - \frac{1}{n^2}\right) + \dots + \frac{b_{2k}}{2k} \left(1 - \frac{1}{n^{2k}}\right) - \int_1^n \frac{B_{2k+1}(\{x\})}{x^{2k+2}} dx. \end{aligned}$$

When $n \rightarrow +\infty$ we get

$$\gamma = \frac{1}{2} + \frac{b_2}{2} + \dots + \frac{b_{2k}}{2k} - \int_1^{+\infty} \frac{B_{2k+1}(\{x\})}{x^{2k+2}} dx.$$

By subtraction, we obtain the equality

$$\gamma = 1 + \frac{1}{2} + \cdots + \frac{1}{n} - \log n - \frac{1}{2n} + \frac{b_2}{2n^2} + \cdots + \frac{b_{2k}}{2kn^{2k}} - \int_n^{+\infty} \frac{B_{2k+1}(\{x\})}{x^{2k+2}} dx.$$

Although this asymptotic expansion is divergent when $k \rightarrow +\infty$, it still gives very good approximations of γ when n and k are well chosen. Indeed, the classical identity

$$B_{2k+1}(\{x\}) = 2(-1)^{k-1}(2k+1)! \sum_{r=1}^{+\infty} \frac{\sin 2r\pi x}{(2r\pi)^{2k+1}}$$

implies

$$|B_{2k+1}(\{x\})| \leq 4 \frac{(2k+1)!}{(2\pi)^{2k+1}},$$

and by means of Stirling's formula, we infer

$$\left| \int_n^{+\infty} \frac{B_{2k+1}(\{x\})}{x^{(2k+2)}} dx \right| \leq \frac{4}{\pi} \left(\frac{k}{n\pi e} \right)^k.$$

Therefore, the remainder term is very small whenever k remains smaller than n .

Analysis of the time complexity.

Let us denote by E_1 this algorithm and by $E_1(d)$ the time complexity for γ with an accuracy of 10^{-d} . We attribute by convention a unit of time to each elementary arithmetic operation on each hardware word of the machine. The sum of two d -digit numbers therefore requires around d units of time, up to a multiplicative constant that will be neglected here; the same is true for products or quotients of multiprecision numbers by "small" numbers represent by one hardware word. A naive evaluation of $1 + \frac{1}{2} + \cdots + \frac{1}{n}$ then requires dn units of time. In practice, one would choose n to be a power of 2 or 10, and $\log n$ itself will be evaluated in d^2 units of time by means of the standard power series $\log 2 = 2 \arg \tanh \frac{1}{3}$ and $\log \frac{10}{8} = 2 \arg \tanh \frac{1}{9}$ that exhibit exponential convergence.

On the other hand, the numbers $\beta_{2k} = \frac{b_{2k}}{n^{2k}}$ can be calculated by means of an induction formula derived from the one satisfied by Bernoulli numbers:

$$\beta_{2k} = \frac{1}{2k+1} \left[\frac{k - \frac{1}{2}}{n^{2k}} - \sum_{j=1}^{k-1} \binom{2k+1}{2j} \frac{\beta_{2j}}{n^{2(k-j)}} \right].$$

The induction step requires about kd units of time, provided that all intermediate terms $\binom{2k+1}{2j} \frac{\beta_{2j}}{n^{2(k-j)}}$ are stored in memory. As a consequence, k^2d units of time are needed to evaluate the sum

$$\frac{b_2}{2n^2} + \cdots + \frac{b_{2k}}{2kn^{2k}}.$$

In total, we obtain a time complexity

$$E_1(d) \sim nd + d^2 + k^2d.$$

Of course, n and k must be chosen so that the error term is $< 10^{-d}$, and this requires

$$k \log \frac{n\pi e}{k} \simeq d \log 10.$$

The optimal choice is obtained for $n \sim k^2$, whence $k \log k \sim d \log 10$, $k \sim \frac{d \log 10}{\log d}$, and

$$E_1(d) \sim Cd^3(\log d)^{-2}.$$

Let us point out that there exists a (lesser known) formula circumventing the calculation of b_{2k} . This formula expresses the remainder in the form of a rapidly convergent double series

$$\gamma = 1 + \frac{1}{2} + \cdots + \frac{1}{n} - \log n - \frac{1}{2n} + \sum_{k=1}^{+\infty} \sum_{\ell=1}^{+\infty} \frac{\ell!}{2^{\ell+1} 2^k n (2^k n + 1) \cdots (2^k n + \ell)}.$$

In order to check this identity, we start from the convergent integral

$$I(p, q) = \int_0^1 x^{p-1} \left(\frac{q}{1-x^q} - \frac{1}{1-x} \right) dx, \quad \text{where } p, q > 0.$$

For every integer $n > 1$, an easy calculation gives

$$I(n, n) = \int_0^1 (1 + x + \cdots + x^{n-1}) dx - d \left[\log \frac{1-x^n}{1-x} \right],$$

so that $I(n, n) = 1 + \frac{1}{2} + \cdots + \frac{1}{n} - \log n \rightarrow \gamma$ when $n \rightarrow +\infty$. The change of variable $x = t^r$ in $I(p, q)$ provides the identity

$$I(p, q) + I(pr, r) = I(pr, qr).$$

Let us apply this formula inductively with $p = q$, $r = 2$. We obtain

$$I(n, n) + I(2n, 2) + \cdots + I(2^k n, 2) = I(2^k n, 2^k n),$$

hence, by taking the limit as $k \rightarrow +\infty$, we get

$$\begin{aligned} \gamma &= I(n, n) + \sum_{k=1}^{+\infty} I(2^k n, 2) \\ &= 1 + \frac{1}{2} + \cdots + \frac{1}{n-1} - \log n + \sum_{k=1}^{+\infty} \int_0^1 x^{2^k n-1} \frac{dx}{1+x}. \end{aligned}$$

The expected formula is then deduced by taking a suitable expansion of $1/(1+x)$:

$$\frac{1}{1+x} = \frac{1}{2} \left(1 - \frac{1-x}{2} \right)^{-1} = \sum_{\ell=0}^{+\infty} \frac{(1-x)^\ell}{2^{\ell+1}}.$$

In particular, for $n = 1$, we obtain the simple formula

$$(E_2) \quad \gamma = \frac{1}{2} + \sum_{k=1}^{+\infty} \sum_{\ell=1}^{+\infty} \frac{\ell!}{2^{\ell+1} 2^k (2^k + 1) \cdots (2^k + \ell)}.$$

The general term of the series is bounded by $\min(2^{-\ell-k-1}, (\ell 2^{-k})^\ell)$; a 10^{-d} accuracy is achieved by performing the summation over indices k, ℓ such that

$$k, \ell \leq d \log 10 / \log 2 \leq 4d, \quad \ell \leq \frac{d \log 10}{k \log 2 - \log \ell}.$$

If we bound ℓ by $4d$ for $k \leq 2 \log(4d) / \log 2$ and by $2d \log 10 / k \log 2$ otherwise, we see that this procedure leaves us with $O(d \log d)$ terms to calculate. Therefore, the time complexity of (E_2) admits the estimate

$$E_2(d) \sim C d^2 \log d,$$

asymptotically smaller than what one obtains with the original (E_1) algorithm. We will see that there actually exist simple $O(d^2)$ algorithms, but the (E_1) algorithm is still probably the most effective one for hand calculations (say, for $d \leq 100$).

2. Sweeney's algorithm

Its starting point is the equality

$$\Gamma'(1) = \int_0^{+\infty} \log t e^t dt = -\gamma,$$

that follows e.g. from the identity of Euler's and Weierstrass' definitions of the Γ function:

$$\Gamma(1+x) = \int_0^{+\infty} t^x e^{-t} dt = e^{-\gamma x} \prod_{n=1}^{+\infty} \left(1 + \frac{x}{n}\right)^{-1}.$$

Through integration by parts, one obtains

$$\gamma = F(x) - \log x - R(x)$$

with

$$F(x) = \int_0^x \frac{1 - e^{-t}}{t} dt,$$

$$R(x) = \int_x^{+\infty} \frac{e^{-t}}{t} dt = \frac{e^{-x}}{x} \left(1 - \frac{1!}{x} + \cdots + \frac{(-1)^k k!}{x^k}\right) + (-1)^{k+1} (k+1)! \int_x^{+\infty} \frac{e^{-t}}{t^{k+2}} dt.$$

The simplest method (S_1) used by Sweeney [21] and Beyer-Waterman [3] is to take an integer x , chosen so big that $R(x)$ is negligible, and to calculate the approximate value $\gamma \simeq F(x) - \log x$. Since $0 < R(x) < \frac{e^{-x}}{x}$, the accuracy 10^{-d} is obtained for $x \simeq d \log 10$.

Given $p \geq 0$, let a_p be the unique positive root of the equation

$$a_p(\log a_p - 1) = p.$$

We have

$$a_0 = e \simeq 2.718, \quad a_1 \simeq 3.591, \quad a_2 \simeq 4.319, \quad a_3 \simeq 4.971.$$

Stirling's formula shows that $\frac{x^n}{n!} \simeq \left(\frac{ex}{n}\right)^n$ is of magnitude e^{-px} for $n \simeq a_p x$. The power series $F(x)$ must be summed up to index $n = \lceil a_1 x \rceil$.

A calculation of the series by means of Hörner's rule

$$F(x) = \frac{x}{1} \left(\frac{1}{1} - \frac{x}{2} \left(\frac{1}{2} - \dots - \frac{x}{n-1} \left(\frac{1}{n-1} - \frac{x}{n} \left(\frac{1}{n} \right) \dots \right) \right) \right),$$

requires 3 arithmetic operations for each term (one multiplication, 1 division, 1 subtraction). An additional difficulty arises here because a certain fraction of the significant digits is lost by compensation of terms of opposite signs. The term of maximum absolute value has an approximate magnitude $\frac{x^n}{n!} \simeq e^x$ for $n = x$, and this requires computing numbers with a precision of $2d$ decimal digits instead of d . Ultimately, one obtains the following computation time (neglecting the evaluation of $\log x$) :

$$S_1(d) = a_1 \times d \log 10 \times 3 \times 2d = 6a_1 \log 10 d^2 \simeq 49.6 d^2.$$

A more elaborate method (S'_1), suggested by Sweeney [21] and implemented by Brent [7], consists in evaluating the remainder $R(x)$ through an asymptotic expansion $R(x)$ truncated at order $k = x \in \mathbb{N}$. Since

$$\left| R(x) - \frac{e^{-x}}{x} \left(1 - \frac{1!}{x} + \dots + \frac{(-1)^k k!}{x^k} \right) \right| \leq \frac{e^{-x} x!}{x^{x+1}} \leq \sqrt{\frac{2\pi}{x}} e^{-2x},$$

one is led to select $x = -\frac{1}{2}d \log 10$, to perform the summation of $F(x)$ up to $n = a_2 x$ ($a_2 \simeq 4.319$), and to work with $\frac{3d}{2}$ digits. Calculating $R(x)$ or e^x requires two steps for each term, evaluated with a precision of $10^{-d/2}$. From this, we infer

$$S'_1(d) = \left(\frac{9}{4} a_2 + \frac{1}{2} a_0 + \frac{1}{2} \right) \log 10 d^2 \simeq 26.7 d^2.$$

There are in fact two alternatives for the calculation of $F(x)$ that avoid the loss of precision by compensation involved in the (S_1) algorithm. They are based on the following developments with positive terms:

$$\begin{aligned} F(x) &= e^{-x} \int_0^x \frac{e^x - e^t}{x-t} dt = e^{-x} \sum_{n=1}^{+\infty} \frac{1}{n!} \int_0^x \frac{x^n - t^n}{x-t} dt \\ (S_2) \quad &= e^{-x} \sum_{n=1}^{+\infty} \left(1 + \frac{1}{2} + \dots + \frac{1}{n} \right) \frac{x^n}{n!} \end{aligned}$$

$$\begin{aligned} F(x) &= e^{-x/2} \int_{-x/2}^{x/2} \frac{e^{x/2} - e^t}{x/2 - t} dt = e^{-x/2} \sum_{n=1}^{+\infty} \frac{1}{n!} \int_{-x/2}^{x/2} \frac{(x/2)^n - t^n}{x/2 - t} dt \\ (S_3) \quad &= e^{-x/2} \sum_{p=1}^{+\infty} 2 \left(1 + \frac{1}{3} + \dots + \frac{1}{2p-1} \right) \left(\frac{(x/2)^{2p-1}}{(2p-1)!} + \frac{(x/2)^{2p}}{(2p)!} \right). \end{aligned}$$

[For this, we use the equality $\frac{x^n - t^n}{x - t} = x^{n-1} + x^{n-2}t + \dots + t^{n-1}$, and for the last summation, we calculate separately at terms $n = 2p$ and $n = 2p - 1$, $p \geq 1$]. The series (S_2), and similarly (S_3), can be evaluated by the following Hörner factorization trick (denoting $H_n = 1 + \frac{1}{2} + \dots + \frac{1}{n}$ the partial sums of the harmonic series, with $H_0 = 0$ by convention, and $H_{n,N} = H_N - H_n = \frac{1}{n+1} + \dots + \frac{1}{N}$):

$$\begin{aligned} e^{-x} \sum_{n=1}^{+\infty} H_n \frac{x^n}{n!} &= H_N - e^{-x} \sum_{n=0}^{+\infty} H_{n,N} \frac{x^n}{n!} \simeq H_N - e^{-x} \sum_{n=0}^{N-1} H_{n,N} \frac{x^n}{n!} \\ &\simeq H_{0,N} - e^{-x} \frac{x}{1} \left(H_{1,N} + \frac{x}{2} \left(H_{2,N} + \frac{x}{3} \left(\dots + \frac{x}{N-1} H_{N-1,N} \right) \dots \right) \right). \end{aligned}$$

The summation is performed from top to bottom, taking inductively $H_{N-1,N} = \frac{1}{N}$ and $H_{n-1,N} = \frac{1}{n} + H_{n,N}$. This requires 1 multiplication, 1 division and 2 additions at each stage. According whether the remainder term $R(x)$ is neglected or not (algorithms including such a remainder will be denoted (S'_2) and (S'_3)), these methods lead to a time complexity

$$\begin{aligned} S_2(d) &= 6a_0 \log 10 d^2 \simeq 37.6 d^2, \\ S_3(d) &= \frac{11}{4} a_1 \log 10 d^2 \simeq 22.7 d^2, \\ S'_2(d) &= \left(3a_1 + \frac{1}{2} \right) \log 10 d^2 \simeq 26.0 d^2, \\ S'_3(d) &= \left(\frac{11}{8} a_3 + \frac{1}{2} \right) \log 10 d^2 \simeq 16.9 d^2. \end{aligned}$$

3. The Brent-McMillan algorithm

This algorithm introduced by Brent-McMillan in [10] is based on certain identities satisfied by the modified Bessel functions $I_\alpha(x)$ and $K_0(x)$:

$$\begin{aligned} I_\alpha(x) &= \sum_{n=0}^{+\infty} \frac{x^{\alpha+2n}}{n! \Gamma(\alpha + n + 1)}, \\ K_0(x) &= - \left. \frac{\partial I_\alpha(x)}{\partial \alpha} \right|_{\alpha=0}. \end{aligned}$$

Experts will observe that $2x$ has been substituted to x in the conventional notation of Watson's treatise [22]. We actually restrict ourselves to values $x > 0$ in what follows. A differentiation of I_α and a use of the formula $\Gamma'(n+1) = (H_n - \gamma) n!$ (the latter being itself a consequence of the equalities $\frac{\Gamma'(x+1)}{\Gamma(x+1)} = \frac{1}{x} + \frac{\Gamma'(x)}{\Gamma(x)}$ and $\Gamma'(1) = -\gamma$) yields

$$\begin{aligned} K_0(x) &= -(\log x + \gamma) I_0(x) + S_0(x) \quad \text{where} \\ I_0(x) &= \sum_{n=0}^{+\infty} \frac{x^{2n}}{n!^2}, \quad S_0(x) = \sum_{n=1}^{+\infty} H_n \frac{x^{2n}}{n!^2}. \end{aligned}$$

The Hankel integral formula expresses the function $1/\Gamma$ as

$$\frac{1}{\Gamma(z)} = \frac{1}{2\pi i} \int_{(C)} \zeta^{-z} e^\zeta d\zeta$$

where (C) is the open contour formed by a small circle $\zeta = \varepsilon e^{iu}$, $u \in [-\pi, \pi]$, concatenated with two half-lines $] -\infty, -\varepsilon]$ with respective arguments $-\pi$ and $+\pi$ and opposite orientation. This formula gives

$$\begin{aligned} I_\alpha(x) &= \sum_{n=0}^{+\infty} \frac{x^{\alpha+2n}}{n!} \frac{1}{2\pi i} \int_{(C)} \zeta^{-\alpha-n-1} e^\zeta d\zeta = \frac{1}{2\pi i} \int_{(C)} x^\alpha \zeta^{-\alpha-1} \exp(x^2/\zeta + \zeta) d\zeta \\ &= \frac{1}{2\pi i} \int_{(C)} \zeta^{-\alpha} \exp(x/\zeta + \zeta x) d\zeta \\ &= \frac{1}{\pi} \int_0^\pi e^{2x \cos u} \cos(\alpha u) du - \frac{\sin \alpha \pi}{\pi} \int_0^{+\infty} e^{-2x \cosh v} e^{-\alpha v} dv. \end{aligned}$$

The integral expressing $I_\alpha(x)$ in the second line above is obtained by means of a change of variable $\zeta \mapsto \zeta x$ (recall that $x > 0$); the first integral of the third line comes from the modified contour consisting of the circle $\{\zeta = e^{iu}\}$ of center 0 and radius 1, and the last integral comes from the corresponding two half-lines $t \in] -\infty, -1]$ written as $t = -e^{-v}$, $v \in]0, +\infty[$. In particular, the following integral expressions and equivalents of $I_0(x)$, $K_0(x)$ hold when $x \rightarrow +\infty$:

$$(1) \quad I_0(x) = \frac{1}{\pi} \int_0^\pi e^{2x \cos u} du \quad \text{hence } I_0(x) \underset{x \rightarrow +\infty}{\sim} \frac{1}{\sqrt{4\pi x}} e^{2x},$$

$$(2) \quad K_0(x) = \int_0^{+\infty} e^{-2x \cosh v} dv \quad \text{hence } K_0(x) \underset{x \rightarrow +\infty}{\sim} \sqrt{\frac{\pi}{4x}} e^{-2x}.$$

Furthermore, one has $I_0(x) > \frac{1}{\sqrt{4\pi x}} e^{2x}$ if $x \geq 1$ and $K_0(x) < \sqrt{\frac{\pi}{4x}} e^{-2x}$ if $x > 0$. These estimates can be checked by means of changes of variables

$$\begin{aligned} I_0(x) &= \frac{e^{2x}}{2\pi\sqrt{x}} \int_0^{4x} \frac{e^{-t}}{\sqrt{t(1-t/4x)}} dt, & t &= 2x(1 - \cos u), \\ K_0(x) &= \frac{e^{-2x}}{2\sqrt{x}} \int_0^{+\infty} \frac{e^{-t}}{\sqrt{t(1+t/4x)}} dt, & t &= 2x(\cosh v - 1), \end{aligned}$$

along with the observation that $\int_0^{+\infty} \frac{1}{\sqrt{t}} e^{-t} dt = \Gamma(\frac{1}{2}) = \sqrt{\pi}$; the lower bound for $I_0(x)$ is obtained by the convexity inequality $\frac{1}{\sqrt{1-t/4x}} \geq 1 + t/8x$ and an integration by parts of the term $\sqrt{t} e^{-t}$, which give

$$\begin{aligned} \int_0^{4x} \frac{e^{-t}}{\sqrt{t(1-t/4x)}} dt &\geq \Gamma(\frac{1}{2}) + \frac{1}{8x} \Gamma(\frac{3}{2}) - \int_{4x}^{+\infty} \left(\frac{1}{\sqrt{t}} + \frac{\sqrt{t}}{8x} \right) e^{-t} dt \\ &\geq \sqrt{\pi} + \frac{\sqrt{\pi}}{16x} - e^{-4x} \left(\frac{3}{4\sqrt{x}} + \frac{1}{32x\sqrt{x}} \right) > \sqrt{\pi} \end{aligned}$$

for $x \geq 1$. As a consequence, Euler's constant can be written as

$$(3) \quad \gamma = \frac{S_0(x)}{I_0(x)} - \log x - \frac{K_0(x)}{I_0(x)},$$

with

$$(4) \quad 0 < \frac{K_0(x)}{I_0(x)} < \pi e^{-4x} \quad \text{if } x \geq 1.$$

In the simpler version (B) of the algorithm proposed by Brent, the remainder $\frac{K_0(x)}{I_0(x)}$ is just neglected ; a precision 10^{-d} is achieved for $x = \frac{1}{4} d \log 10$, and the power series $I_0(x)$, $S_0(x)$ must be summed up to $n = \lceil a_1 x \rceil$. The calculation of

$$I_0(x) = 1 + \frac{x^2}{1^2} \left(1 + \frac{x^2}{2^2} \left(\cdots \frac{x^2}{(n-1)^2} \left(1 + \frac{x^2}{n^2} \left(\cdots \right) \right) \cdots \right) \right)$$

requires 2 arithmetic operations for each term, and that of

$$S_0(x) \simeq H_{0,N} - \frac{1}{I_0(x)} \frac{x^2}{1^2} \left(H_{1,N} + \frac{x^2}{2^2} \left(\cdots \frac{x^2}{(n-1)^2} \left(H_{n-1,N} + \frac{x^2}{n^2} \left(H_{n,N} + \cdots \right) \right) \cdots \right) \right)$$

requires 4 operations. The time required by the algorithm (B) is thus

$$B(d) = a_1 \times \frac{1}{4} d \log 10 \times 6 \times d \simeq 12.4 d^2.$$

Refinement of the algorithm. As in the case of Sweeney's method, the remainder term $K_0(x)/I_0(x)$ can be evaluated by means of an asymptotic expansion. In fact

$$I_0(x)K_0(x) = \frac{1}{2\pi} \int_{\{-\pi < u < \pi, v > 0\}} \exp(2x(\cos u - \cosh v)) du dv,$$

and a change of variables

$$r e^{i\theta} = \sin^2 \left(\frac{u + iv}{2} \right) = \frac{1}{2} (1 - \cos(u + iv)) = \frac{1}{2} (1 - \cos u \cosh v + i \sin u \sinh v)$$

gives

$$\begin{aligned} r &= \frac{1}{2} (\cosh v - \cos u), & |1 - r e^{i\theta}| &= \left| \cos \left(\frac{u + iv}{2} \right) \right|^2, \\ r dr d\theta &= \left| \sin \left(\frac{u + iv}{2} \right) \cos \left(\frac{u + iv}{2} \right) \right|^2 du dv = r |1 - r e^{i\theta}| du dv, \end{aligned}$$

therefore

$$(5) \quad I_0(x)K_0(x) = \frac{1}{2\pi} \int_0^{+\infty} \exp(-4xr) dr \int_0^{2\pi} \frac{d\theta}{|1 - r e^{i\theta}|}.$$

Let us denote

$$\binom{\alpha}{k} = \frac{\alpha(\alpha-1)\cdots(\alpha-k+1)}{k!}, \quad \alpha \in \mathbb{C}$$

the (generalized) binomial coefficients. For $z = r e^{i\theta}$ and $|z| = r < 1$ the binomial identity $(1-z)^{-1/2} = \sum_{k=0}^{+\infty} \binom{-\frac{1}{2}}{k} (-z)^k$ combined with the Parseval-Bessel formula yields the expansion

$$(6) \quad \varphi(r) := \frac{1}{2\pi} \int_0^{2\pi} \frac{d\theta}{|1 - r e^{i\theta}|} = \sum_{k=0}^{+\infty} w_k r^{2k}, \quad 0 \leq r < 1,$$

where the coefficient

$$(7) \quad w_k := \binom{-1/2}{k}^2 = \left(\frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2 \cdot 4 \cdot 6 \cdots 2k} \right)^2 = \frac{(2k)!^2}{2^{4k} k!^4}.$$

is closely related to the Wallis integral $W_p = \int_0^{\pi/2} \sin^p x \, dx$. Indeed, the easily established induction relation $W_p = \frac{p-1}{p} W_{p-2}$ implies

$$W_{2k} = \frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2 \cdot 4 \cdot 6 \cdots 2k} \frac{\pi}{2}, \quad W_{2k+1} = \frac{2 \cdot 4 \cdot 6 \cdots 2k}{3 \cdot 5 \cdots (2k+1)},$$

whence $w_k = \left(\frac{2}{\pi} W_{2k}\right)^2$. The relations $W_{2k} W_{2k-1} = \frac{\pi}{4k}$, $W_{2k} W_{2k+1} = \frac{\pi}{2(2k+1)}$ together with the monotonicity of (W_p) imply that $\sqrt{\frac{\pi}{2(2k+1)}} < W_{2k} < \sqrt{\frac{\pi}{4k}}$, therefore

$$(8) \quad \frac{2}{\pi(2k+1)} < w_k < \frac{1}{\pi k}.$$

The starting point of our analysis for estimating $I_0(x)K_0(x)$ is the following integral formula derived from (5), (6):

$$(9) \quad I_0(x)K_0(x) = \int_0^{+\infty} e^{-4xr} \varphi(r) \, dr,$$

where

$$(9') \quad \varphi(r) = \sum_{k=0}^{+\infty} w_k r^{2k} \quad \text{for } r < 1,$$

$$(9'') \quad \varphi(r) = \frac{1}{r} \varphi\left(\frac{1}{r}\right) = \sum_{k=0}^{+\infty} w_k r^{-2k-1} \quad \text{for } r > 1.$$

(The last identity can be seen immediately by applying the change of variable $\theta \mapsto -\theta$ in (6)). It is also easily checked using (8) that one has an equivalent

$$\varphi(r) \sim \sum_{k=1}^{+\infty} \frac{r^{2k}}{\pi k} = \frac{1}{\pi} \log \frac{1}{1-r^2} \quad \text{when } r \rightarrow 1-0,$$

in particular the integral (9) converges near $r = 1$ (later, we will need a more precise approximation relying on more sophisticated arguments). By an integration term by term on $[0, +\infty[$ of the series defining $\varphi(r)$, and by ignoring the fact that the series diverges for $r \geq 1$, one formally obtains a (divergent) asymptotic expansion

$$(10) \quad I_0(x)K_0(x) \sim \sum_{k \in \mathbb{N}} w_k \frac{(2k)!}{(4x)^{2k+1}} \sim \frac{1}{4x} \sum_{k \in \mathbb{N}} \frac{(2k)!^3}{k!^4 (16x)^{2k}}.$$

If x is an integer, the general term of this expansion achieves its minimum exactly for $k = 2x$, since the ratio of the k -th and $(k-1)$ -st terms is

$$\frac{(2k(2k-1))^3}{k^4 (16x)^2} = \left(\frac{k}{2x}\right)^2 \left(1 - \frac{1}{2k}\right)^3 < 1 \quad \text{iff } k \leq 2x.$$

The idea is to truncate the asymptotic expansion precisely at $k = 2x$. We will check, as was conjectured by Brent-McMillan [10] and partly proven by Brent and Johansson [10'] that the corresponding "truncation error" is then of an order of magnitude comparable to that of last term $k = 2x$ involved, namely $\frac{e^{-4x}}{2\sqrt{2\pi}x^{3/2}}$ by the Stirling formula.

Theorem. *The truncation error*

$$(11) \quad \Delta(x) := I_0(x)K_0(x) - \frac{1}{4x} \sum_{k=0}^{2x} \frac{(2k)!^3}{k!^4 (16x)^{2k}}$$

admits when $x \rightarrow +\infty$ an equivalent

$$(12) \quad \Delta(x) \sim -\frac{5e^{-4x}}{24\sqrt{2\pi}x^{3/2}},$$

and more specifically

$$(13) \quad \Delta(x) = -e^{-4x} \left(\frac{5}{24\sqrt{2\pi}x^{3/2}} + \varepsilon(x) \right), \quad |\varepsilon(x)| < \frac{0.863}{x^2}.$$

The approximate value

$$\frac{K_0(x)}{I_0(x)} \simeq \frac{1}{4x I_0(x)^2} \sum_{k=0}^{2x} \frac{(2k)!^3}{k!^4 (16x)^{2k}}$$

is thus affected by an error of magnitude

$$(13') \quad \frac{\Delta(x)}{I_0(x)^2} \sim -\frac{5\sqrt{2\pi}}{12x^{1/2}} e^{-8x}.$$

The proof of this result requires many calculations. The discussion made below would probably even yield an asymptotic development for $\Delta(x)$, at least for the first few terms, but the required calculations would probably be quite long. By (5) and the definition of $\Delta(x)$ we have

$$(14) \quad \Delta(x) = \int_0^{+\infty} e^{-4xr} \delta(r) dr$$

where

$$(15) \quad \delta(r) := \varphi(r) - \sum_{k=0}^{2x} w_k r^{2k}, \quad \text{so that} \quad \delta(r) = \sum_{k=2x+1}^{+\infty} w_k r^{2k} \quad \text{for} \quad r < 1.$$

For $r < 1$, let us observe that $\varphi(r)$ coincides with the elliptic integral of the first kind $\frac{2}{\pi} \int_0^{\pi/2} (1-r^2 \sin^2 \theta)^{-1/2} d\theta$, as follows again from the binomial formula and the expression of W_{2k} . We need to calculate the precise asymptotic behavior of $\varphi(r)$ when $r \rightarrow 1$. This

can be obtained by means of a well known identity which we recall below. By putting $t^2 = 1 - r^2$, the change of variable $u = \tan \theta$ gives

$$\begin{aligned} \varphi(r) &= \frac{2}{\pi} \int_0^{\pi/2} (1 - r^2 \cos^2 \theta)^{-1/2} d\theta = \frac{2}{\pi} \int_0^{+\infty} \frac{du}{\sqrt{(1+u^2)(t^2+u^2)}} du \\ (16) \quad &= \frac{4}{\pi} \int_0^1 \frac{dv}{\sqrt{(1+v^2)(1+t^2v^2)}} + \frac{2}{\pi} \int_t^1 \frac{dv}{\sqrt{(1+v^2)(t^2+v^2)}} \end{aligned}$$

where the last line is obtained by splitting the integral $\int_0^{+\infty} \dots du$ on the 3 intervals $[0, t]$, $[t, 1]$, $[1, +\infty[$, and by performing the respective changes of variable $u = vt, u = v$, $u = 1/v$ (the first and third pieces being then equal). Thanks to the binomial formula, the first integral of line (16) admits a development as a convergent series

$$\frac{4}{\pi} \int_0^1 \frac{dv}{\sqrt{(1+v^2)(1+t^2v^2)}} = \frac{4}{\pi} \sum_{k=0}^{+\infty} c'_k t^{2k}, \quad c'_k = \binom{-1/2}{k} \int_0^1 \frac{v^{2k} dv}{\sqrt{1+v^2}}.$$

The second integral can be expressed as the sum of a double series when we simultaneously expand both square roots :

$$\frac{2}{\pi} \int_t^1 \frac{dv}{v\sqrt{1+v^2} \sqrt{(1+t^2/v^2)}} = \frac{2}{\pi} \int_t^1 \sum_{k, \ell \geq 0} \binom{-1/2}{\ell} v^{2\ell} \binom{-1/2}{k} (t^2/v^2)^k \frac{dv}{v}.$$

The diagonal part $k = \ell$ yields a logarithmic term

$$\frac{2}{\pi} \sum_{k=0}^{+\infty} \binom{-1/2}{k}^2 t^{2k} \log \frac{1}{t} = \frac{1}{\pi} \varphi(t) \log \frac{1}{t^2},$$

and the other terms can be collected in the form of an absolutely convergent double series

$$\frac{2}{\pi} \sum_{k \neq \ell \geq 0} \binom{-1/2}{k} \binom{-1/2}{\ell} t^{2k} \left[\frac{v^{2\ell-2k}}{2\ell-2k} \right]_t^1 = \frac{2}{\pi} \sum_{k \neq \ell \geq 0} \binom{-1/2}{k} \binom{-1/2}{\ell} \frac{t^{2k} - t^{2\ell}}{2(\ell - k)}.$$

After grouping the various powers t , the summation reduces to a power series $\frac{4}{\pi} \sum c''_k t^{2k}$ of radius of convergence 1, where (due to the symmetry in k, ℓ)

$$c''_k = \sum_{0 \leq \ell < +\infty, \ell \neq k} \frac{1}{2(\ell - k)} \binom{-1/2}{k} \binom{-1/2}{\ell}.$$

In fact, we see a priori from (8) that

$$|c'_k| \leq \frac{1}{\sqrt{\pi k}} \frac{1}{2k+1} = O(k^{-3/2}),$$

and

$$|c''_k| \leq \frac{1}{2\sqrt{\pi k}} \left(\frac{1}{k} + \sum_{0 < \ell \neq k} \frac{1}{|\ell - k| \sqrt{\pi \ell}} \right) = O\left(\frac{\log k}{k}\right).$$

In total, if we put $t^2 = 1 - r^2$, the above relation implies

$$(17) \quad \varphi(r) = \frac{1}{\pi} \left(\varphi(t) \log \frac{1}{t^2} + 4 \sum_{k=0}^{+\infty} c_k t^{2k} \right), \quad c_k = c'_k + c''_k,$$

and this identity will produce an arbitrarily precise expansion of $\varphi(r)$ when $r \rightarrow 1$. In order to compute the coefficients, we observe that

$$c_k = c'_k + c''_k = \binom{-1/2}{k} \alpha_k$$

with

$$\alpha_k = \int_0^1 \frac{v^{2k} dv}{\sqrt{1+v^2}} + \int_1^{+\infty} \left(\frac{v^{2k}}{\sqrt{1+v^2}} - \sum_{\ell=0}^k \binom{-1/2}{\ell} v^{2k-2\ell-1} \right) dv + \sum_{\ell=0}^{k-1} \frac{1}{2(\ell-k)} \binom{-1/2}{\ell}.$$

A direct calculation gives

$$c_0 = \alpha_0 = \int_0^1 \frac{dv}{\sqrt{1+v^2}} + \int_1^{+\infty} \left(\frac{1}{\sqrt{1+v^2}} - \frac{1}{v} \right) dv = \log 2.$$

Next, if we write

$$\frac{v^{2k}}{\sqrt{1+v^2}} = v^{2k-1} \cdot \frac{v}{\sqrt{1+v^2}}, \quad (\sqrt{1+v^2})' = \frac{v}{\sqrt{1+v^2}}$$

and integrate by parts after factoring v^{2k-1} , we get

$$\begin{aligned} \alpha_k &= \sum_{\ell=0}^{k-1} \frac{1}{2(\ell-k)} \binom{-1/2}{\ell} + \left[v^{2k-1} \sqrt{1+v^2} \right]_0^1 - \int_0^1 (2k-1) v^{2k-2} \sqrt{1+v^2} dv \\ &\quad + \left[v^{2k-1} \left(\sqrt{1+v^2} - \sum_{\ell=0}^k \binom{-1/2}{\ell} \frac{v^{1-2\ell}}{1-2\ell} \right) \right]_1^{+\infty} \\ &\quad - \int_1^{+\infty} (2k-1) v^{2k-2} \left(\sqrt{1+v^2} - \sum_{\ell=0}^k \binom{-1/2}{\ell} \frac{v^{1-2\ell}}{1-2\ell} \right) dv. \end{aligned}$$

This suggests to calculate $\alpha_k + (2k-1)\alpha_{k-1}$ and to use the simplification

$$v^{2k-2} \sqrt{1+v^2} - \frac{v^{2k-2}}{\sqrt{1+v^2}} = \frac{v^{2k}}{\sqrt{1+v^2}}.$$

We then infer

$$\begin{aligned} \alpha_k + (2k-1)\alpha_{k-1} &= -(2k-1)\alpha_k + \sum_{\ell=0}^k \binom{-1/2}{\ell} \frac{1}{1-2\ell} \\ &\quad + \int_1^{+\infty} (2k-1) v^{2k-2} \left(\sum_{\ell=0}^k \binom{-1/2}{\ell} \left(\frac{v^{1-2\ell}}{1-2\ell} - v^{1-2\ell} \right) - \sum_{\ell=0}^{k-1} \binom{-1/2}{\ell} v^{-1-2\ell} \right) dv \\ &\quad + 2k \sum_{\ell=0}^{k-1} \frac{1}{2(\ell-k)} \binom{-1/2}{\ell} + (2k-1) \sum_{\ell=0}^{k-2} \frac{1}{2(\ell-(k-1))} \binom{-1/2}{\ell}. \end{aligned}$$

A change of indices $\ell = \ell' - 1$ in the sums corresponding to $k - 1$ then eliminates almost all terms. There only remains the term $\ell = k$ in the first summation, whence the induction relation

$$2k \alpha_k + (2k - 1)\alpha_{k-1} = -\binom{-1/2}{k} \frac{1}{2k - 1}, \quad \text{i.e.} \quad \frac{\alpha_k}{\binom{-1/2}{k}} - \frac{\alpha_{k-1}}{\binom{-1/2}{k-1}} = -\frac{1}{2k(2k - 1)}.$$

We get in this way

$$\frac{c_k}{\binom{-1/2}{k}^2} = \frac{\alpha_k}{\binom{-1/2}{k}} = \frac{\alpha_0}{1} - \sum_{\ell=1}^k \frac{1}{2\ell(2\ell - 1)} = \log 2 - \sum_{\ell=1}^{2k} \frac{(-1)^{\ell-1}}{\ell}$$

and the explicit expression

$$(18) \quad c_k = w_k \left(\log 2 - \sum_{\ell=1}^{2k} \frac{(-1)^{\ell-1}}{\ell} \right).$$

The remainder of the alternating series expressing $\log 2$ is bounded by half of last calculated term, namely $1/4k$, thus according to (8) we have $0 < c_k < \frac{1}{\pi^2 k^2}$ if $k \geq 1$, and the radius of convergence of the series is 1. From (9) and (17) we infer as $r \rightarrow 1 - 0$ the well known expansion of the elliptic integral

$$(19) \quad \varphi(r) = \frac{1}{\pi} \left(\sum_{k=0}^{+\infty} w_k t^{2k} \log \frac{1}{t^2} + 4 \sum_{k=0}^{+\infty} c_k t^{2k} \right), \quad t^2 = 1 - r^2,$$

with

$$w_0 = 1, \quad w_1 = \frac{1}{4}, \quad w_2 = \frac{9}{64}, \quad c_0 = \log 2, \quad c_1 = \frac{1}{4} \left(\log 2 - \frac{1}{2} \right), \quad c_2 = \frac{9}{64} \left(\log 2 - \frac{7}{12} \right).$$

Let us compute explicitly the first terms of the asymptotic expansion at $r = 1$ by putting $r = 1 + h$, $h \rightarrow 0$. For $r = 1 + h < 1$ ($h < 0$) we have $t^2 = 1 - r^2 = -2h - h^2 = 2|h|(1 + h/2)$, where

$$\begin{aligned} \log \frac{1}{t^2} &= \log \frac{1}{2|h|(1 + h/2)} = \log \frac{1}{|h|} - \log 2 - \frac{1}{2}h + \frac{1}{8}h^2 + O(h^2), \\ \sum_{k=0}^{+\infty} w_k t^{2k} &= 1 + \frac{1}{4}(-2h - h^2) + \frac{9}{64}(2h)^2 + O(h^3), \\ 4 \sum_{k=0}^{+\infty} c_k t^{2k} &= 4 \log 2 + \left(\log 2 - \frac{1}{2} \right)(-2h - h^2) + \frac{9}{16} \left(\log 2 - \frac{7}{12} \right)(2h)^2 + O(h^3), \end{aligned}$$

and

$$\begin{aligned} \varphi(1 + h) &= \frac{1}{\pi} \left(\left(1 - \frac{1}{2}h + \frac{5}{16}h^2 + O(h^3) \right) \left(\log \frac{1}{|h|} - \log 2 - \frac{1}{2}h + \frac{1}{8}h^2 + O(h^3) \right) \right. \\ &\quad \left. + 4 \log 2 - (2 \log 2 - 1)h + \left(\frac{5}{4} \log 2 - \frac{13}{16} \right)h^2 + O(h^3) \right). \end{aligned}$$

If terms are written by decreasing order of magnitude, we get

$$(20) \quad \varphi(1+h) = \frac{1}{\pi} \left(\log \frac{1}{|h|} + 3 \log 2 - \frac{1}{2} h \log \frac{1}{|h|} - \left(\frac{3}{2} \log 2 - \frac{1}{2} \right) h \right. \\ \left. + \frac{5}{16} h^2 \log \frac{1}{|h|} + \left(\frac{15}{16} \log 2 - \frac{7}{16} \right) h^2 + O\left(h^3 \log \frac{1}{|h|} \right) \right).$$

For $r = 1 + h > 1$, the identity $\varphi(r) = \frac{1}{r} \varphi\left(\frac{1}{r}\right)$ gives in a similar way

$$\varphi(r) = \frac{1}{1+h} \left(\frac{1}{\pi} \sum_{k=0}^{+\infty} w_k t^{2k} \log \frac{1}{t^2} + \sum_{k=0}^{+\infty} c_k t^{2k} \right), \quad t^2 = 1 - \frac{1}{r^2} = 2h - 3h^2 + O(h^3).$$

After a few simplifications, one can see that the expansion (20) is still valid for $h > 0$. Passing to the limit $r \rightarrow 0$, $t \rightarrow 1 - 0$ in (19) implies the relation $\sum_{k \geq 0} c_k = \frac{\pi}{4}$. The following Lemma will be useful.

Lemma 1. *For $h > 0$ the difference*

$$(21) \quad \rho(h) = \varphi(1+h) - \frac{1}{\pi} \left(\log \frac{1}{h} + 3 \log 2 - \frac{1}{2} h \log \frac{1}{h} - \left(\frac{3}{2} \log 2 - \frac{1}{2} \right) h \right)$$

$$(21') \quad = \varphi(1+h) - \frac{1}{2\pi} \left((h-2) \log \frac{h}{8} + h \right)$$

admits the upper bound

$$(22) \quad |\rho(h)| \leq h^2 \left(2 + \log \left(1 + \frac{1}{h} \right) \right).$$

Proof. A use of the Taylor-Lagrange formula gives $(1+h)^{-1} = 1 - h + \theta_1 h^2$, $t^2 = 1 - \frac{1}{r^2} = 2h - 3\theta_2 h^2$, with $\theta_i \in]0, 1[$, and we also find $t^2 \leq 2h$ and

$$\log \frac{1}{t^2} = \log \frac{r^2}{(r-1)(r+1)} = \log \frac{1}{h} + 2 \log(1+h) - \log \left(1 + \frac{h}{2} \right) - \log 2 \\ = \log \frac{1}{h} - \log 2 + \frac{3}{2} h - \frac{7}{8} \theta_3 h^2, \quad \theta_2 \in]0, 1[$$

while the remainder terms $\sum_{k \geq 2} w_k t^{2k}$ and $\sum_{k \geq 2} c_k t^{2k}$ are bounded respectively by

$$\frac{w_2 t^4}{1-t^2} \leq 4w_2 r^2 h^2 \leq \frac{225}{256} h^2 \quad \text{and} \quad \frac{c_2 t^4}{1-t^2} \leq 4c_2 r^2 h^2 < \frac{1}{10} h^2 \quad \text{if } h \leq \frac{1}{4}, r = 1+h \leq \frac{5}{4}.$$

For $h \leq \frac{1}{4}$ we thus get an equality

$$\varphi(1+h) = \frac{1}{\pi} (1 - h + \theta_1 h^2) \times \left(\left(1 + \frac{1}{4} (2h - 3\theta_2 h^2) + \frac{225}{256} \theta_4 h^2 \right) \left(\log \frac{1}{|h|} - \log 2 + \frac{3}{2} h - \frac{7}{8} \theta_3 h^2 \right) \right. \\ \left. + 4 \log 2 + \left(\log 2 - \frac{1}{2} \right) (2h - 3\theta_2 h^2) + \frac{4}{10} \theta_5 h^2 \right)$$

with $\theta_i \in]0, 1[$. In order to estimate $\rho(h)$, we fully expand this expression and replace each term by an upper bound of its absolute value. For $h \leq \frac{1}{4}$, this shows that $|\rho(h)| \leq h^2(0.885 \log \frac{1}{h} + 2.11)$, so that (22) is satisfied. For $h \geq \frac{1}{4}$, we write

$$\rho'(h) = \varphi'(1+h) - \frac{1}{2\pi} \left(\log \frac{h}{8} + 2 - \frac{2}{h} \right), \quad \varphi'(r) = - \sum_{k=0}^{+\infty} (2k+1) w_k r^{-2k-2},$$

and by (8) we get

$$\sum_{k=0}^{+\infty} \frac{2}{\pi} r^{-2k-2} < -\varphi'(r) < \frac{1}{r^2} + \sum_{k=1}^{+\infty} \frac{3k}{\pi k} r^{-2k-2} < \sum_{k=0}^{+\infty} r^{-2k-2} = \frac{1}{r^2-1},$$

therefore

$$\begin{aligned} \frac{2}{\pi} \frac{1}{h(h+2)} < -\varphi'(1+h) < \frac{1}{h(h+2)}, \\ \frac{1}{2\pi} \left(\log \frac{8}{h} - 2 + \frac{2}{h} - \frac{2\pi}{h(h+2)} \right) < \rho'(h) < \frac{1}{2\pi} \left(\log \frac{8}{h} - 2 + \frac{2}{h+2} \right). \end{aligned}$$

This implies

$$\begin{aligned} -1.72 < \frac{1}{2\pi} \left(\log 4 - 2 + \frac{1}{4} - \frac{32\pi}{9} \right) < \rho'(h) < \frac{1}{2\pi} \left(\log 32 - 2 + \frac{8}{9} \right) < 1.51 \quad \text{on } \left[\frac{1}{4}, 2 \right], \\ -\frac{1}{2\pi} \left(\log \frac{h}{8} + 2 \right) < \rho'(h) < \frac{1}{2\pi} \left(\log 4 - \frac{3}{2} \right) < 0 \quad \text{on } [2, +\infty[, \end{aligned}$$

therefore $|\rho'(h)| \leq \frac{1}{2\pi}(h-1-\log 8+2) \leq \frac{1}{2\pi}h$ for $h \in [2, +\infty[$. Since $\rho(2) \simeq 0.00249 < \frac{1}{\pi}$, we see that $|\rho(h)| \leq \frac{1}{4\pi}h^2$, and this shows that (22) still holds on $[2, +\infty[$. A numerical calculation of $\rho(h)$ at sufficiently close points in the interval $[\frac{1}{4}, 2]$ finally yields (22) on that interval. \square

Now we split the integral (14) on the intervals $[0, 1]$ and $[1, +\infty[$, starting with the integral of φ on the interval $[1, +\infty[$. The change of variable $r = 1 + t/4x$ provides

$$(23) \quad \int_1^{+\infty} e^{-4xr} \varphi(r) dr = \frac{e^{-4x}}{4x} \int_0^{+\infty} e^{-t} \varphi\left(1 + \frac{t}{4x}\right) dt,$$

and Lemma 1 (21') yields for this integral an approximation

$$\begin{aligned} & \frac{e^{-4x}}{8\pi x} \int_0^{+\infty} e^{-t} \left(\left(\frac{t}{4x} - 2 \right) \log \frac{t}{32x} + \frac{t}{4x} \right) dt \\ &= \frac{e^{-4x}}{8\pi x} \left(\log(32x) \left(2 - \frac{1}{4x} \right) + 2\gamma + \frac{1}{4x} \int_0^{+\infty} e^{-t} (t \log t + t) dt \right) \\ &= \frac{e^{-4x}}{4\pi x} \left(\log x + \gamma + 5 \log 2 - \frac{\log x}{8x} - \frac{\gamma + 5 \log 2 - 2}{8x} \right), \end{aligned}$$

with an error bounded by

$$\begin{aligned} \frac{e^{-4x}}{4x} \int_0^{+\infty} e^{-t} \left(\frac{t}{4x} \right)^2 \left(2 + \log \left(1 + \frac{4x}{t} \right) \right) dt \\ = \frac{e^{-4x}}{4x} \left(\frac{1}{4x^2} + \frac{1}{16x^2} \int_0^{+\infty} t^2 e^{-t} \log \frac{t+4x}{t} dt \right). \end{aligned}$$

Writing

$$0 < \log \frac{t+4x}{t} = \log \frac{4x}{t} + \log \left(1 + \frac{t}{4x} \right) \leq \log \frac{4x}{t} + \frac{t}{4x},$$

we further see that

$$\int_0^{+\infty} t^2 e^{-t} \log \frac{t+4x}{t} dt \leq \int_0^{+\infty} t^2 e^{-t} \left(\log \frac{4x}{t} + \frac{t}{4x} \right) dt = 2 \log 4x + \frac{3}{2x} + 2\gamma - 3.$$

We infer

$$(24) \quad \int_1^{+\infty} e^{-4xr} \varphi(r) dr = \frac{e^{-4x}}{4\pi x} \left(\log x + \gamma + 5 \log 2 - \frac{\log x}{8x} \right) + \frac{e^{-4x}}{4x} R_1(x),$$

and a numerical calculation shows that

$$(25) \quad |R_1(x)| < \frac{\gamma + 5 \log 2 - 2}{8\pi x} + \frac{1}{4x^2} + \frac{2 \log 4x + \frac{3}{2x} + 2}{16x^2} < \frac{0.483}{x}.$$

We now estimate the two integrals $\int_0^1 e^{-4xr} \sum_{k \geq 2x+1} w_k r^{2k} dr$, $\int_1^{+\infty} e^{-4xr} \sum_{k \leq 2x} w_k r^{2k} dr$.

Thanks to iterated integrations by parts, we get

$$(26) \quad \int_0^1 e^{-4xr} r^{2k} dr = e^{-4x} \sum_{\ell=1}^{+\infty} \frac{(4x)^{\ell-1}}{(2k+1) \cdots (2k+\ell)},$$

$$(27) \quad \int_1^{+\infty} e^{-4xr} r^{2k} dr = \frac{e^{-4x}}{4x} \left(1 + \sum_{\ell=1}^{2k} \frac{2k(2k-1) \cdots (2k-\ell+1)}{(4x)^\ell} \right).$$

Combining the identities (14), (15), (24), (26), (27) we find

$$(28) \quad \Delta(x) = \frac{e^{-4x}}{4x} \left(\frac{1}{\pi} \left(\log x + \gamma + 5 \log 2 \right) - \frac{\log x}{8\pi x} - \sum_{k=0}^{2x} w_k + S(x) + R_1(x) + R_2(x) \right)$$

with

$$(29) \quad S(x) = \sum_{k=2x+1}^{+\infty} \sum_{\ell=1}^{2x-1} \frac{w_k (4x)^\ell}{(2k+1) \cdots (2k+\ell)} - \sum_{k=1}^{2x} \sum_{\ell=1}^{2x-1} w_k \frac{2k(2k-1) \cdots (2k-\ell+1)}{(4x)^\ell},$$

and

$$(30) \quad R_2(x) = \sum_{k=2x+1}^{+\infty} \sum_{\ell=2x}^{+\infty} \frac{w_k (4x)^\ell}{(2k+1) \cdots (2k+\ell)} - \sum_{k=1}^{2x} \sum_{\ell=2x}^{+\infty} w_k \frac{2k(2k-1) \cdots (2k-\ell+1)}{(4x)^\ell}$$

(In the final summation, terms of index $\ell > 2k$ are zero). Formula (28) leads us to study the asymptotic expansion of $\sum_{k=0}^{2x} w_k$. This development is easy to establish from (19) (one could even calculate it at an arbitrarily large order).

Lemma 2. *One has*

$$(31) \quad w_k = \frac{1}{\pi k} \left(1 - \frac{1}{2(2k-1)} + \varepsilon_k \right) \quad \text{where} \quad \frac{1}{12k(2k-1)} < \varepsilon_k < \frac{5}{16k(2k-1)}, \quad k \geq 1,$$

$$(31') \quad \sum_{k=0}^{2x} w_k = \frac{1}{\pi} \left(\log x + 5 \log 2 + \gamma \right) + R_3(x), \quad \frac{1}{4\pi x} < R_3(x) < \frac{19}{48\pi x}.$$

Proof. The lower bound (31) is a consequence of the Euler-Maclaurin's formula of §1 applied to the function $f(x) = \log \frac{2x-1}{2x}$. This yields

$$\frac{1}{2} \log w_k = \sum_{i=1}^k f(i) = C + \int_1^k f(x) dx + \frac{1}{2} f(k) + \sum_{j=1}^p \frac{b_{2j}}{(2j)!} f^{(2j-1)}(k) + \tilde{R}_p$$

where C is a constant, and where the remainder term \tilde{R}_p is the product of the next term by a factor $[0, 1]$, namely

$$\frac{b_{2p+2}}{(2p+2)!} f^{(2p+1)}(k) = \frac{2^{2p+1} b_{2p+2}}{(2p+1)(2p+2)} \left(\frac{1}{(2k-1)^{2p+1}} - \frac{1}{(2k)^{2p+1}} \right).$$

We have here

$$\begin{aligned} \int_1^k f(x) dx &= \frac{1}{2} (2k-1) \log(2k-1) - k \log k - (k-1) \log 2 \\ &= \left(k - \frac{1}{2} \right) \log \left(1 - \frac{1}{2k} \right) - \frac{1}{2} \log k + \frac{1}{2} \log 2 \end{aligned}$$

and the constant C can be computed by the Wallis formula. Therefore, with $b_2 = \frac{1}{6}$, we have

$$\begin{aligned} \log w_k &= \log \frac{1}{\pi k} + 2k \log \left(1 - \frac{1}{2k} \right) + 1 + 2\theta b_2 \left(\frac{1}{(2k-1)} - \frac{1}{2k} \right) \\ &\geq \log \frac{1}{\pi k} - \frac{1}{4k} - \sum_{\ell=3}^{+\infty} \frac{1}{\ell(2k)^\ell} > \log \frac{1}{\pi k} - \frac{1}{4k} - \frac{1}{3} \frac{1}{(2k)^2} \frac{1}{1 - \frac{1}{2k}}. \end{aligned}$$

The inequality $e^{-x} \geq 1 - x$ then gives

$$w_k > \frac{1}{\pi k} \left(1 - \frac{1}{4k} - \frac{1}{6k(2k-1)} \right) = \frac{1}{\pi k} \left(1 - \frac{1}{2(2k-1)} + \frac{1}{12k(2k-1)} \right)$$

and the lower bound (31) follows for all $k \geq 1$. In the other direction, we get

$$\log w_k < \log \frac{1}{\pi k} - \frac{1}{4k} - \frac{1}{12k^2} - \frac{1}{32k^3} + \frac{1}{6k(2k-1)} = \log \frac{1}{\pi k} - \frac{1}{4k} + \frac{1}{12k^2(2k-1)} - \frac{1}{32k^3}$$

and the inequality $e^{-x} \leq 1 - x + \frac{1}{2}x^2$ implies

$$w_k < \frac{1}{\pi k} \left(1 - \left(\frac{1}{4k} - \frac{1}{12k^2(2k-1)} + \frac{1}{32k^3} \right) + \frac{1}{2} \left(\frac{1}{4k} \right)^2 \right)$$

whence (by a difference of polynomials and a reduction to the same denominator)

$$w_k < \frac{1}{\pi k} \left(1 - \frac{1}{2(2k-1)} + \frac{5}{16k(2k-1)} \right) \quad \text{if } k \geq 3.$$

One can check that the final inequality still holds for $k = 1, 2$, and this implies the estimate (31). On the other hand, formula (19) yields

$$\begin{aligned} w_0 + \sum_{k=1}^{+\infty} \left(w_k - \frac{1}{\pi k} \right) r^{2k} &= \varphi(r) - \frac{1}{\pi} \log \frac{1}{1-r^2} \\ &= \frac{1}{\pi} (\varphi(t) - 1) \log \frac{1}{1-r^2} + \frac{4}{\pi} \log 2 + \sum_{k \geq 1} c_k t^{2k} \end{aligned}$$

with $t = \sqrt{1-r^2}$ and $\varphi(t) = 1 + O(1-r^2)$. By passing to the limit when $r \rightarrow 1-0$ and $t \rightarrow 0$, we thus get

$$w_0 + \sum_{k=1}^{+\infty} \left(w_k - \frac{1}{\pi k} \right) = \frac{4}{\pi} \log 2.$$

We infer

$$w_0 + \sum_{k=1}^{2x} \left(w_k - \frac{1}{\pi k} \right) - \frac{4}{\pi} \log 2 = \sum_{2x+1}^{+\infty} \left(\frac{1}{\pi k} - w_k \right)$$

and the upper and lower bounds in (31) imply

$$0 < \sum_{2x+1}^{+\infty} \left(\frac{1}{\pi k} - w_k \right) \leq \sum_{2x+1}^{+\infty} \frac{1}{2\pi k(2k-1)} < \sum_{2x+1}^{+\infty} \frac{1}{4\pi} \frac{1}{k(k-1)} = \frac{1}{8\pi x}.$$

The Euler-Maclaurin estimate

$$(32) \quad \sum_{k=1}^{2x} \frac{1}{k} = \log(2x) + \gamma + \frac{1}{4x} + \frac{b_2}{2(2x)^2} - \frac{b_4}{4(2x)^4} + \dots$$

then finally yields (31'). □

It remains to evaluate the sum $S(x)$. This is considerably more difficult, as a consequence of a partial cancellation of positive and negative terms. The approximation (31) obtained in Lemma 2 implies

$$(33) \quad S(x) = \frac{2}{\pi} \left(T(x) - \frac{1}{2}U(x) + \frac{5}{8}R_4(x) \right),$$

and if we agree as usual that the empty product $(2k-2) \cdots (2k-\ell+1) = \frac{1}{2k-1}$ for $\ell = 1$ is equal to 1, we get

$$(34) \quad T(x) = \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell}{2k(2k+1) \cdots (2k+\ell)} - \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-1) \cdots (2k-\ell+1)}{(4x)^\ell},$$

$$(35) \quad U(x) = \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell}{(2k-1) \cdots (2k+\ell)} - \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-2) \cdots (2k-\ell+1)}{(4x)^\ell},$$

where the new error term $R_4(x)$ admits the upper bound

$$(36) \quad |R_4(x)| \leq \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell/2k}{(2k-1) \cdots (2k+\ell)} + \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-2) \cdots (2k-\ell+1)}{2k(4x)^\ell}.$$

Our method consists in performing first a summation over the index k , and for this, we use “discrete integrations by parts”. Let us set

$$(37) \quad u_k^{a,b} := \frac{1}{(2k+a)(2k+a+1) \cdots (2k+b-1)}, \quad a \leq b$$

(agreeing that the denominator is 1 if $a = b$). Then

$$\begin{aligned} u_k^{a,b} - u_{k+1}^{a,b} &= \frac{(2k+b)(2k+b+1) - (2k+a)(2k+a+1)}{(2k+a)(2k+a+1) \cdots (2k+b+1)} \\ &= \frac{(b-a)(4k+a+b+1)}{(2k+a)(2k+a+1) \cdots (2k+b+1)}. \end{aligned}$$

The inequalities $2(2k+a) \leq 4k+a+b+1 \leq 2(2k+b+1)$ imply

$$\frac{1}{(2k+a+1) \cdots (2k+b+1)} \leq \frac{u_k^{a,b} - u_{k+1}^{a,b}}{2(b-a)} \leq \frac{1}{(2k+a)(2k+a+1) \cdots (2k+b)}$$

with an upward error and a downward error both equal to

$$\frac{b-a+1}{2} \frac{1}{(2k+a)(2k+a+1) \cdots (2k+b+1)}.$$

In particular, through a summation $\sum_{k=2x+1}^{+\infty} \frac{u_k^{a-1,b-1} - u_{k+1}^{a-1,b-1}}{2(b-a)}$, these inequalities imply

$$\sum_{k=2x+1}^{+\infty} \frac{1}{(2k+a) \cdots (2k+b)} \leq \frac{u_{2x+1}^{a-1,b-1}}{2(b-a)} = \frac{1}{2(b-a)} \frac{1}{(4x+a+1) \cdots (4x+b)},$$

with an upward error equal to

$$\frac{b-a+1}{2} \sum_{k=2x+1}^{+\infty} \frac{1}{(2k+a-1) \cdots (2k+b)} \leq \frac{1}{4} \frac{1}{(4x+a) \cdots (4x+b)}$$

and an “error on the error” (again upwards) equal to

$$\frac{(b-a+1)(b-a+2)}{4} \sum_{k=2x+1}^{+\infty} \frac{1}{(2k+a-2)\cdots(2k+b)} \leq \frac{b-a+1}{8} \frac{1}{(4x+a-1)\cdots(4x+b)}.$$

In other words, we find

$$\begin{aligned} \sum_{k=2x+1}^{+\infty} \frac{1}{(2k+a)\cdots(2k+b)} &= \frac{1}{2(b-a)} \frac{1}{(4x+a+1)\cdots(4x+b)} - \frac{1}{4} \frac{1}{(4x+a)\cdots(4x+b)} \\ (38_3^{a,b}) \quad &+ \theta \frac{b-a+1}{8} \frac{1}{(4x+a-1)\cdots(4x+b)}, \quad \theta \in [0, 1]. \end{aligned}$$

If necessary, one could of course push further this development to an arbitrary number of terms p rather than 3. We will denote the corresponding expansion $(37_p^{a,b})$, and will use it here in the cases $p = 2, 3$. For the summations $\sum_{k=1}^{2x} \dots$, we similarly define

$$(39) \quad v_k^{a,b} = (2k-a)(2k-a-1)\cdots(2k-b+1), \quad a \leq b,$$

and obtain

$$\begin{aligned} v_k^{a,b} - v_{k-1}^{a,b} &= (2k-a-2)\cdots(2k-b+1)((2k-a)(2k-a-1) - (2k-b)(2k-b-1)) \\ &= (2k-a-2)\cdots(2k-b+1)((b-a)(4k-a-b-1)). \end{aligned}$$

For $a < b$, the inequalities $2(2k-b) \leq (4k-a-b-1) \leq 2(2k-a-1)$ imply

$$(2k-a-2)\cdots(2k-b) \leq \frac{v_k^{a,b} - v_{k-1}^{a,b}}{2(b-a)} \leq (2k-a-1)\cdots(2k-b+1)$$

with an upward error and a downward error both equal to

$$\frac{1}{2}(b-a-1)(2k-a-2)\cdots(2k-b+1).$$

By considering the sum $\sum_{k=1}^{2x} \frac{v_k^{a,b} - v_{k-1}^{a,b}}{2(b-a)}$, we obtain

$$\sum_{k=1}^{2x} (2k-a-1)\cdots(2k-b+1) \geq \frac{v_{2x}^{a,b} - v_0^{a,b}}{2(b-a)}$$

with a downward error

$$\frac{b-a-1}{2} \sum_{k=1}^{2x} (2k-a-2)\cdots(2k-b+1) \leq \frac{v_{2x}^{a,b-1} - v_0^{a,b-1}}{4}$$

and an upward error on the error equal to

$$\frac{(b-a-1)(b-a-2)}{4} \sum_{k=1}^{2x} (2k-a-2)\cdots(2k-b+2) \leq \frac{b-a-1}{8} (v_{2x}^{a,b-2} - v_0^{a,b-2}),$$

i.e. there exists $\theta \in [0, 1]$ such that

$$\begin{aligned} & \sum_{k=1}^{2x} (2k-a-1) \cdots (2k-b+1) \\ &= \frac{1}{2(b-a)} (v_{2x}^{a,b} - v_0^{a,b}) + \frac{1}{4} (v_{2x}^{a,b-1} - v_0^{a,b-1}) - \theta \frac{b-a-1}{8} (v_{2x}^{a,b-2} - v_0^{a,b-2}), \\ (40_3^{a,b}) \quad &= \frac{1}{2(b-a)} v_{2x}^{a,b} + \frac{1}{4} v_{2x}^{a,b-1} - \theta \frac{b-a-1}{8} v_{2x}^{a,b-2} + C_3^{a,b}, \end{aligned}$$

with

$$(41_3^{a,b}) \quad |C_3^{a,b}| \leq \frac{1}{2(b-a)} |v_0^{a,b}| + \frac{1}{4} |v_0^{a,b-1}| + \frac{b-a-1}{8} |v_0^{a,b-2}|,$$

especially $C_3^{a,b} = 0$ if $a = 0$. The simpler order 2 case (with an initial error by excess) gives

$$\begin{aligned} & \sum_{k=1}^{2x} (2k-a-2) \cdots (2k-b) = \frac{1}{2(b-a)} (v_{2x}^{a,b} - v_0^{a,b}) - \theta \frac{1}{4} (v_{2x}^{a,b-1} - v_0^{a,b-1}) \\ (40_2^{a,b}) \quad &= \frac{1}{2(b-a)} (4x-a) \cdots (4x-b+1) - \theta \frac{1}{4} (4x-a) \cdots (4x-b+2) + C_2^{a,b}. \end{aligned}$$

In the order 3 case, it will be convenient to use a further change

$$v_k^{a,b} - v_k^{a+1,b+1} = (2k-a-1) \cdots (2k-b+1) \left((2k-a) - (2k-b) \right) = (b-a) v_k^{a+1,b}.$$

If we apply this equality to the values (a, b) , $(a, b-1)$ and $k = 2x$, we see that the $(40_3^{a,b})$ development can be written in the equivalent form

$$\begin{aligned} & \sum_{k=1}^{2x} (2k-a-1) \cdots (2k-b+1) - C_3^{a,b} \\ &= \frac{1}{2(b-a)} v_{2x}^{a+1,b+1} + \frac{3}{4} v_{2x}^{a+1,b} + \frac{b-a-1}{8} \left(2 v_{2x}^{a+1,b-1} - \theta v_{2x}^{a,b-2} \right), \\ &= \frac{1}{2(b-a)} (4x-a-1) \cdots (4x-b) + \frac{3}{4} (4x-a-1) \cdots (4x-b+1) \\ (\widetilde{40}_3^{a,b}) \quad &+ \frac{b-a-1}{8} \left(2(4x-a-1) \cdots (4x-b+2) - \theta (4x-a) \cdots (4x-b+3) \right) \end{aligned}$$

According to (34), $(38_3^{0,\ell})$ and $(\widetilde{40}_3^{0,\ell})$, we get

$$(42) \quad T(x) = T'(x) - T''(x) + R_5(x)$$

with

$$(43) \quad T'(x) = \sum_{\ell=1}^{2x-1} \frac{1}{2\ell} \left(\frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} - \frac{(4x-1) \cdots (4x-\ell)}{(4x)^\ell} \right),$$

$$(43') \quad T''(x) = \sum_{\ell=1}^{2x-1} \frac{1}{4} \frac{(4x)^\ell}{4x(4x+1) \cdots (4x+\ell)} + \frac{3}{4} \frac{(4x-1) \cdots (4x-\ell+1)}{(4x)^\ell},$$

$$(43'') \quad |R_5(x)| \leq \frac{1}{8} \sum_{\ell=1}^{2x-1} \left(\frac{(\ell+1)(4x)^\ell}{(4x-1)4x \cdots (4x+\ell)} + \frac{2(\ell-1)(4x-1) \cdots (4x-\ell+2)}{(4x)^\ell} \right).$$

The last term in the last line comes from formula $(\widetilde{40}_3^{0,\ell})$, by observing that the inequalities $4x \leq 2(4x - \ell + 2)$ $\ell \leq 2x - 1$ imply

$$4x(4x - 1) \cdots (4x - \ell + 3) \leq 2(4x - 1) \cdots (4x - \ell + 2).$$

Similarly, thanks to (35), $(38_2^{-1,\ell})$ and $(40_2^{0,\ell-1})$, we obtain the decomposition

$$(44) \quad U(x) = U'(x) - U''(x) + R_6(x)$$

with

$$(45) \quad U'(x) = \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)} \frac{(4x)^\ell}{4x \cdots (4x + \ell)} - \sum_{\ell=2}^{2x-1} \frac{1}{2(\ell-1)} \frac{4x(4x-1) \cdots (4x-\ell+2)}{(4x)^\ell},$$

$$(45') \quad U''(x) = \frac{1}{4x} \sum_{k=1}^{2x} \frac{1}{2k-1} \quad (\text{negative term } \ell = 1 \text{ appearing in } U(x)),$$

$$(45'') \quad |R_6(x)| \leq \frac{1}{4} \sum_{\ell=1}^{2x-1} \frac{(4x)^\ell}{(4x-1) \cdots (4x+\ell)} + \frac{1}{4} \sum_{\ell=2}^{2x-1} \frac{4x(4x-1) \cdots (4x-\ell+3)}{(4x)^\ell}.$$

The remainder terms $R_2(x)$ [resp. $R_4(x)$] can be bounded in the same way by means of $(38_2^{0,\ell})$ and $(40_2^{-1,\ell-1})$ [resp. $(38_2^{-1,\ell})$ and $(40_2^{0,\ell-2})$] and (8), (30), (36) lead to

$$|R_2(x)| \leq \frac{2}{\pi} \left(\sum_{\ell=2x}^{+\infty} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell}{(2k) \cdots (2k+\ell)} + \sum_{\ell=2x}^{+\infty} \sum_{k=1}^{2x} \frac{(2k-1) \cdots (2k-\ell+1)}{(4x)^\ell} \right)$$

$$(46) \quad \leq \frac{2}{\pi} \sum_{\ell=2x}^{+\infty} \frac{1}{2\ell} \left(\frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} + \frac{(4x+1) \cdots (4x-\ell+2)}{(4x)^\ell} \right),$$

$$|R_4(x)| \leq \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^{\ell-1}}{(2k-1) \cdots (2k+\ell)} + \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-2) \cdots (2k-\ell+2)}{(4x)^\ell}$$

$$(46') \quad \leq \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)} \frac{(4x)^{\ell-1}}{4x \cdots (4x+\ell)} + \sum_{\ell=3}^{2x-1} \frac{1}{2(\ell-2)} \frac{4x(4x-1) \cdots (4x-\ell+3)}{(4x)^\ell}$$

$$(46'') \quad + \sum_{k=1}^{2x} \frac{1}{2k(2k-1)} \frac{1}{4x} + \sum_{k=1}^{2x} \frac{1}{(2k-1)} \frac{1}{(4x)^2} \quad [\text{terms } \ell = 1, 2 \text{ in the summation}].$$

Finally, by (28), (31'), (33) and (42), (44) we get the decomposition

$$(47) \quad \Delta(x) = \frac{e^{-4x}}{4\pi x} \left(2T'(x) - 2T''(x) - U'(x) + U''(x) - \frac{\log x}{8x} \right. \\ \left. + \pi \left(R_1(x) + R_2(x) - R_3(x) \right) - \frac{5}{4} R_4(x) + 2R_5(x) - R_6(x) \right).$$

Lemma 3. *The following inequalities hold:*

$$(48) \quad \log 2 - \frac{1}{8x} < \sum_{k=1}^{2x} \frac{1}{2k(2k-1)} < \log 2 - \frac{1}{2(4x+1)},$$

$$(48') \quad \sum_{k=1}^{2x} \frac{1}{2k-1} < \frac{3}{2} \log 2 + \frac{1}{2} (\log x + \gamma) + \frac{1}{24x^2},$$

$$(48'') \quad U''(x) = \frac{\log x}{8x} + R_7(x), \quad 0 < R_7(x) < \frac{1.37}{x}.$$

Proof. To check (48), we observe that the sum of the series is $\log 2$ and that the remainder of index $2x$ admits the lower and upper bounds

$$\begin{aligned} \frac{1}{2(4x+1)} &= \sum_{k=2x+1}^{+\infty} \frac{1}{4} \left(\frac{1}{k-1/2} - \frac{1}{k+1/2} \right) \\ &< \sum_{k=2x+1}^{+\infty} \frac{1}{2k(2k-1)} < \sum_{k=2x+1}^{+\infty} \frac{1}{4} \left(\frac{1}{k-1} - \frac{1}{k} \right) = \frac{1}{8x}. \end{aligned}$$

According to the Euler-Maclaurin expansion (32), we get on the one hand

$$\begin{aligned} \sum_{k=1}^{2x} \frac{1}{2k-1} &= \sum_{\ell=1}^{4x} \frac{(-1)^{\ell-1}}{\ell} + \sum_{\ell=1}^{2x} \frac{1}{2\ell} = \sum_{k=1}^{2x} \frac{1}{2k(2k-1)} + \frac{1}{2} \sum_{k=1}^{2x} \frac{1}{k} \\ &< \log 2 - \frac{1}{2(4x+1)} + \frac{1}{2} \left(\log(2x) + \gamma + \frac{1}{4x} + \frac{1}{12(2x)^2} \right) \\ &= \frac{3}{2} \log 2 + \frac{1}{2} (\log x + \gamma) + \frac{1}{8x(4x+1)} + \frac{1}{96x^2}, \end{aligned}$$

whence (48'), and on the other hand

$$\begin{aligned} \sum_{k=1}^{2x} \frac{1}{2k-1} &> \log 2 + \frac{1}{2} \left(\log(2x) + \gamma + \frac{1}{12(2x)^2} - \frac{1}{120(2x)^4} \right) \\ &> \frac{3}{2} \log 2 + \frac{1}{2} (\log x + \gamma) + \frac{1}{96x^2} - \frac{1}{1920x^4}. \end{aligned}$$

A straightforward numerical computation gives $\frac{3}{2} \log 2 + \frac{1}{2} \gamma + \frac{1}{24} < 1.37$, which then yields (48''). \square

We will now check that all remainder terms $R_i(x)$ are of a lower order of magnitude than the main terms, and in particular that they admit a bound $O(1/x)$. The easier term to estimate is $R_6(x)$. One can indeed use a very rough inequality

$$(49) \quad |R_6(x)| \leq \frac{1}{4} \sum_{\ell=1}^{2x-1} \frac{1}{4x(4x-1)} + \frac{1}{4} \sum_{\ell=2}^{2x-1} \frac{1}{(4x)^2} \leq \frac{1}{4} \frac{2x-1}{4x(4x-1)} + \frac{1}{4} \frac{2x-2}{(4x)^2} < \frac{1}{16x}.$$

Consider now $R_4(x)$. We use Lemma 3 to bound both summations appearing in (46''), and get in this way

$$[[(46'')]] \leq \frac{\log 2 - \frac{1}{2(4x+1)}}{4x} + \frac{\frac{3}{2} \log 2 + \frac{1}{2}(\log x + \gamma) + \frac{1}{24x^2}}{(4x)^2} < \frac{0.234}{x}$$

(this is clear for x large since $\frac{1}{4} \log 2 < 0.234$ – the precise check uses a direct numerical calculation for smaller values of x). By even more brutal estimates, we find

$$\begin{aligned} \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)} \frac{(4x)^{\ell-1}}{4x \cdots (4x+\ell)} &\leq \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)} \frac{1}{(4x)^2} \leq \frac{\log 2x + \gamma + \frac{1}{4x} + \frac{1}{12(2x)^2} - 1}{32x^2} < \frac{0.025}{x}, \\ \sum_{\ell=3}^{2x-1} \frac{1}{2(\ell-2)} \frac{4x(4x-1) \cdots (4x-\ell+1)}{(4x)^{\ell+2}} &\leq \sum_{\ell=1}^{2x-3} \frac{1}{\ell} \frac{1}{32x^2} \leq \frac{\log 2x + \gamma}{32x^2} < \frac{0.040}{x}. \end{aligned}$$

This gives the final estimate

$$(50) \quad |R_4(x)| \leq \frac{0.299}{x}.$$

In order to get an optimal bound of the other terms, we must more precisely estimate the partial products $\prod(4x \pm j)$, and for this, we use the power series expansion of the logarithm function. For $t > 0$, we have $t - \frac{1}{2}t^2 < \log(1+t) < t$. By taking $t = \frac{j}{4x}$, we find

$$-\frac{\sum_{1 \leq j \leq \ell} j}{4x} < \log \frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} = \sum_{1 \leq j \leq \ell} \log \frac{1}{1 + \frac{j}{4x}} < -\frac{\sum_{1 \leq j \leq \ell} j}{4x} + \frac{\sum_{1 \leq j \leq \ell} j^2}{2(4x)^2}.$$

Since $\sum_{1 \leq j \leq \ell} j = \frac{\ell(\ell+1)}{2}$ and $\sum_{1 \leq j \leq \ell} j^2 = \frac{\ell(\ell+1)(2\ell+1)}{6}$, we get

$$-\frac{\ell(\ell+1)}{8x} < \log \frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} < -\frac{\ell(\ell+1)}{8x} + \frac{\ell(\ell+1)(2\ell+1)}{12(4x)^2},$$

therefore

$$(51) \quad \exp\left(\frac{1}{32x} - \frac{(\ell+1/2)^2}{8x}\right) < \frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} < \exp\left(\frac{1}{32x} - \frac{(\ell+1/2)^2}{8x} + \frac{(\ell+1/2)^3}{96x^2}\right).$$

For $\ell \leq 2x - 1$ we have

$$\frac{(\ell+1/2)^2}{8x} - \frac{(\ell+1/2)^3}{96x^2} = \frac{(\ell+1/2)^2}{8x} \left(1 - \frac{(\ell+1/2)}{12x}\right) \geq \frac{5}{6} \frac{(\ell+1/2)^2}{8x},$$

hence (after performing a suitable numerical calculation)

$$(51') \quad \begin{aligned} \frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} &< \exp\left(\frac{1}{32x} - \frac{5}{6} \frac{(\ell+1/2)^2}{8x}\right) && \text{for } \ell \leq 2x - 1, \\ \frac{(4x)^\ell}{(4x+1) \cdots (4x+\ell)} &< \exp\left(\frac{1}{32x} - \frac{5}{6} \frac{(2x-1/2)^2}{12x}\right) < \frac{1.52}{x} && \text{for } \ell \geq 2x - 1. \end{aligned}$$

For $\ell \geq 2x$, each new factor is at most $\frac{4x}{4x+\ell} \leq \frac{2}{3}$, thus

$$(51'') \quad \sum_{\ell=2x}^{+\infty} \frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} < \frac{1.52}{x} \sum_{p=1}^{+\infty} \left(\frac{2}{3}\right)^p < \frac{3.04}{x}.$$

On the other hand, the analogous inequality $-t - 16t^2/26 < \log(1-t) < -t$ applied with $t = \frac{j}{4x} \leq 1/4$ implies

$$(52) \quad -\frac{\ell(\ell+1)}{8x} - \frac{16\ell(\ell+1)(2\ell+1)}{6 \cdot 26(4x)^2} < \log \frac{(4x-1)\cdots(4x-\ell)}{(4x)^\ell} < -\frac{\ell(\ell+1)}{8x}.$$

As $\exp(1/4x) > 1 + 1/4x$, we infer

$$(52') \quad \frac{(4x+1)\cdots(4x-\ell+2)}{(4x)^\ell} \leq \left(1 + \frac{1}{4x}\right) \exp\left(-\frac{(\ell-1)(\ell-2)}{8x}\right) < \exp\left(-\frac{\ell(\ell-3)}{8x}\right),$$

and the ratio of two consecutive upper bounds associated with indices $\ell, \ell+1$ is less than $\exp(-(2\ell-2)/8x) \leq e^{-1/4}$ if $\ell = 2x$ and less than $e^{-1/2}$ if $\ell \geq 2x+1$, thus

$$\sum_{\ell=2x}^{+\infty} \frac{(4x+1)\cdots(4x-\ell+2)}{(4x)^\ell} \leq \exp\left(\frac{3}{4} - \frac{x}{2}\right) \left(1 + e^{-1/4} \sum_{p=0}^{+\infty} e^{-p/2}\right) < \frac{4.65}{x}.$$

As $2\ell \geq 4x$, we deduce from (46) that

$$(53) \quad |R_2(x)| \leq \frac{2}{\pi} \frac{1}{4x} \frac{7.69}{x} < \frac{1.224}{x^2}$$

(but actually, one can see that $R_2(x)$ even decays exponentially). By means of a standard integral-series comparison, the inequalities (43''), (51') and (52') also provide

$$(54) \quad \begin{aligned} |R_5(x)| &\leq \frac{1}{8} \sum_{\ell=1}^{2x-1} \frac{\ell+1}{4x(4x-1)} \exp\left(\frac{1}{32x} - \frac{5}{6} \frac{(\ell+1/2)^2}{8x}\right) + 2 \frac{\ell-1}{(4x)^2} \exp\left(\frac{3\ell}{8x} - \frac{\ell^2}{8x}\right) \\ &\leq \frac{1}{8(4x)(3x)} \left(e^{\frac{1}{32}} \int_0^{+\infty} \left(t + \frac{3}{2}\right) \exp\left(-\frac{5}{6} \frac{t^2}{8x}\right) dt + \frac{3e^{\frac{3}{4}}}{2} \int_0^{+\infty} t \exp\left(-\frac{t^2}{8x}\right) dt \right) \\ &= \frac{1}{96x^2} \left(e^{\frac{1}{32}} \left(\frac{24}{5}x + \frac{3}{2} \sqrt{\frac{48x}{5}} \frac{1}{2} \sqrt{\pi} \right) + 6e^{\frac{3}{4}}x \right) < \frac{0.229}{x} \quad \text{for } x \geq 1. \end{aligned}$$

It then follows from (43) and (51) that

$$\begin{aligned} T'(x) &= \sum_{\ell=1}^{2x-1} \frac{1}{2\ell} \left(\frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} - \frac{(4x-1)\cdots(4x-\ell)}{(4x)^\ell} \right) \\ &= \sum_{\ell=1}^{2x-1} \frac{1}{2\ell} \frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} \left(1 - \prod_{j=1}^{\ell} \left(1 - \frac{j}{4x}\right) \left(1 + \frac{j}{4x}\right) \right) \\ &\leq \sum_{\ell=1}^{2x-1} \exp\left(\frac{1}{32x} - \frac{(\ell+1/2)^2}{8x} + \frac{(\ell+1/2)^3}{96x^2}\right) \frac{(\ell+1)^2}{96x^2}; \end{aligned}$$

to get this, we have used here the inequality $1 - \prod(1 - a_j) \leq \sum a_j$ with $a_j = \frac{j^2}{(4x)^2} < 1$, and the identity $\sum_{j \leq \ell} j^2 = \frac{\ell(\ell+1)(2\ell+1)}{6}$. In the other direction, we have a lower bound $\prod(1 - a_j)^{-1} - 1 \geq \sum a_j$, thus (52) implies

$$\begin{aligned} T'(x) &= \sum_{\ell=1}^{2x-1} \frac{1}{2\ell} \frac{(4x-1) \cdots (4x-\ell)}{(4x)^\ell} \left(\prod_{j=1}^{\ell} \left(1 - \left(\frac{j}{4x} \right)^2 \right)^{-1} - 1 \right) \\ &\geq \sum_{\ell=1}^{2x-1} \exp \left(-\frac{\ell(\ell+1)}{8x} - \frac{(\ell+1/2)^3}{78x^2} \right) \frac{(\ell+1)(2\ell+1)}{12(4x)^2} \\ &\geq \sum_{\ell=1}^{2x-1} \exp \left(-\frac{(\ell+1/2)^2}{8x} - \frac{(\ell+1/2)^3}{78x^2} \right) \frac{(\ell+1)(\ell+1/2)}{96x^2} \\ &\geq \sum_{\ell=1}^{2x-1} \exp \left(-\frac{(\ell+1/2)^2}{8x} \right) \left(1 - \frac{(\ell+1/2)^3}{78x^2} \right) \frac{(\ell+1)(\ell+1/2)}{96x^2}. \end{aligned}$$

We now evaluate these sums by comparing them to integrals. This gives

$$T'(x) \leq e^{\frac{1}{32x}} \int_0^{2x} \exp \left(-\frac{t^2}{8x} + \frac{t^3}{96x^2} \right) \frac{(t+3/2)^2}{96x^2} dt$$

when we estimate the term of index ℓ by the corresponding integral on the interval $[\ell - 1/2, \ell + 1/2]$. The change of variable

$$u = \frac{t^2}{8x} - \frac{t^3}{96x^2} = \frac{t^2}{8x} \left(1 - \frac{t}{12x} \right), \quad du = \frac{t}{4x} \left(1 - \frac{t}{8x} \right) dt$$

implies $u \geq \frac{5}{48x} t^2$, hence $t \leq \sqrt{\frac{48x}{5}} \sqrt{u}$. Moreover, a trivial convexity argument yields $(1 - \frac{v}{p})^{-1} \leq 1 + \frac{1}{p-1} v$ if $v \leq 1$; if we take $v = \frac{t}{2x}$ and $p = 6$ (resp. $p = 3$), we find

$$\begin{aligned} t &= \sqrt{8xu} \left(1 - \frac{t}{12x} \right)^{-1/2} \leq \sqrt{8xu} \left(1 + \frac{t}{20x} \right) \leq \sqrt{8xu} \left(1 + \sqrt{\frac{3}{125x}} \sqrt{u} \right), \\ dt &= \frac{4x}{t} \left(1 - \frac{t}{8x} \right)^{-1} du \leq \frac{4x}{t} \left(1 + \frac{t}{6x} \right) du \leq \frac{4x}{\sqrt{8xu}} \left(1 + \frac{2}{\sqrt{15x}} \sqrt{u} \right) du, \end{aligned}$$

therefore

$$T'(x) \leq \frac{e^{\frac{1}{32x}}}{96x^2} \int_0^{+\infty} e^{-u} \left(\frac{3}{2} + \sqrt{8xu} \left(1 + \sqrt{\frac{3}{125x}} \sqrt{u} \right) \right)^2 \left(1 + \frac{2}{\sqrt{15x}} \sqrt{u} \right) \frac{\sqrt{2x} du}{\sqrt{u}}.$$

This integral can be evaluated explicitly, its dominant term being equal to

$$\frac{e^{\frac{1}{32x}}}{96x^2} \int_0^{+\infty} e^{-u} (\sqrt{8xu})^2 \frac{\sqrt{2x} du}{\sqrt{u}} \sim \frac{\sqrt{2}}{12\sqrt{x}} \int_0^{+\infty} e^{-u} \sqrt{u} du = \frac{\sqrt{2\pi}}{24x^{1/2}}.$$

Moreover, the factor $e^{\frac{1}{32x}}$ factor admits the (very rough!) upper bound $1 + \frac{1}{31.5x}$, whence an error bounded by

$$\frac{\sqrt{2\pi}}{24x^{1/2}} \cdot \frac{1}{31.5x} < \frac{0.004}{x}.$$

All other terms appearing in the integral involve terms $O(\frac{1}{x})$ with coefficients which are products of factors $\Gamma(a)$, $\frac{1}{2} \leq a \leq 2$, by coefficients whose sum is bounded by

$$\frac{e^{\frac{1}{32}}}{96} \left[\left(\frac{3}{2} + \sqrt{8} \left(1 + \sqrt{\frac{3}{125}} \right) \right)^2 \left(1 + \frac{2}{\sqrt{15}} \right) \sqrt{2} - 8\sqrt{2} \right] < 0.4021.$$

As $\Gamma(a) \leq \sqrt{\pi}$, we obtain

$$T'(x) < \frac{\sqrt{2\pi}}{24x^{1/2}} + \frac{0.717}{x}.$$

Similarly, one can obtain the following lower bound for $T'(x)$:

$$\begin{aligned} T'(x) &\geq \sum_{\ell=1}^{2x-1} \exp\left(-\frac{(\ell+1/2)^2}{8x}\right) \left(1 - \frac{(\ell+1/2)^3}{78x^2}\right) \frac{(\ell+1)(\ell+1/2)}{96x^2} \\ &\geq \int_{3/2}^{2x+1/2} \exp\left(-\frac{t^2}{8x}\right) \left(1 - \frac{t^3}{78x^2}\right) \frac{(t-1)(t-1/2)}{96x^2} dt \\ &\geq \int_2^{2x} \exp\left(-\frac{t^2}{8x}\right) \left(1 - \frac{t^3}{78x^2}\right) \frac{t^2 - 3t/2}{96x^2} dt \\ &= \int_{1/2x}^{x/2} e^{-u} \left(1 - \frac{8\sqrt{8}u^{3/2}}{78x^{1/2}}\right) \frac{8xu - 3\sqrt{8}x^{1/2}u^{1/2}/2}{96x^2} \frac{\sqrt{8}x^{1/2}du}{2u^{1/2}} \\ &\geq \int_{1/2x}^{x/2} e^{-u} \left(1 - \frac{8\sqrt{8}u^{3/2}}{78x^{1/2}}\right) \frac{\sqrt{8}u - 3x^{-1/2}u^{1/2}/2}{24x^{1/2}} \frac{du}{u^{1/2}} \\ &\geq \int_{1/2x}^{x/2} e^{-u} \left(\frac{\sqrt{2}u^{1/2}}{12x^{1/2}} - \frac{8u^2}{3 \cdot 78x} - \frac{1}{16x}\right) du \\ &\geq \int_0^{+\infty} e^{-u} \left(\frac{\sqrt{2}u^{1/2}}{12x^{1/2}} - \frac{4u^2}{117x} - \frac{1}{16x}\right) du - \int_{\mathfrak{C}} e^{-u} \frac{\sqrt{2}u^{1/2}}{12x^{1/2}} du. \end{aligned}$$

The integral $\int_{\mathfrak{C}} \dots$ on the “missing intervals” is bounded on $[0, 1/2x]$ by

$$\int_0^{1/2x} \frac{\sqrt{2}u^{1/2}}{12x^{1/2}} du = \frac{1}{36x^2},$$

whilst the integral on $[A, +\infty[= [x/2, +\infty[$ satisfies

$$\int_A^{+\infty} u^\alpha e^{-u} du = A^\alpha e^{-A} + \int_A^{+\infty} \alpha u^{\alpha-1} e^{-u} du \leq e^{-A}(A^\alpha + \alpha A^{\alpha-1}), \quad \alpha \in]0, 1].$$

This provides an estimate

$$\int_{\frac{x}{2}}^{+\infty} e^{-u} \frac{\sqrt{2}u^{1/2}}{12x^{1/2}} du \leq \exp\left(-\frac{x}{2}\right) \left(\frac{1}{12} + \frac{1}{12x}\right) \leq \frac{1}{6} \frac{e^{-1/2}}{x}.$$

Therefore, we obtain the explicit lower bound

$$T'(x) > \frac{\sqrt{2\pi}}{24x^{1/2}} - \left(\frac{8}{117} + \frac{1}{16} + \frac{1}{36} + \frac{1}{6}e^{-1/2} \right) \frac{1}{x} > \frac{\sqrt{2\pi}}{24x^{1/2}} - \frac{0.260}{x}.$$

In the same manner, but now without any compensation of terms and with much simpler calculations, the estimates (43''), (51), (52) provide an upper bound

$$T''(x) \leq \frac{1}{4x} \sum_{\ell=1}^{2x-1} \frac{1}{4} \exp\left(\frac{32}{x} - \frac{(\ell+1/2)^2}{8x} + \frac{(\ell+1/2)^3}{96x^2}\right) + \frac{3}{4} \exp\left(\frac{32}{x} - \frac{(\ell-1/2)^2}{8x}\right).$$

By using integral estimates very similar to those already used, this gives

$$\begin{aligned} T''(x) &\leq \frac{e^{\frac{32}{x}}}{4x} \left(\frac{1}{4} \int_0^{2x} \exp\left(-\frac{t^2}{8x} + \frac{t^3}{96x^2}\right) dt + \frac{3}{4} \int_0^{2x} \exp\left(-\frac{t^2}{8x}\right) dt \right) + \frac{3}{16x} \\ &\leq \frac{e^{\frac{32}{x}}}{4x} \left(\frac{1}{4} \int_0^{+\infty} e^{-u} \left(1 + \frac{2}{\sqrt{15x}} \sqrt{u}\right) \frac{\sqrt{2x} du}{\sqrt{u}} + \frac{3}{4} \int_0^{+\infty} e^{-u} \frac{\sqrt{2x} du}{\sqrt{u}} \right) + \frac{3}{16x} \\ &\leq \frac{e^{\frac{32}{x}}}{4x} \int_0^{+\infty} e^{-u} \frac{\sqrt{2x} du}{\sqrt{u}} + \frac{e^{\frac{32}{x}}}{4x} \frac{1}{\sqrt{30}} + \frac{3}{16x} < \frac{\sqrt{2\pi}}{4x^{1/2}} + \frac{0.255}{x}, \end{aligned}$$

and we get likewise a lower bound

$$\begin{aligned} T''(x) &\geq \frac{1}{4x} \sum_{\ell=1}^{2x-1} \frac{1}{4} \exp\left(-\frac{(\ell+1/2)^2}{8x}\right) + \frac{3}{4} \exp\left(-\frac{(\ell-1/2)^2}{8x} - \frac{(\ell-1/2)^3}{78x^2}\right) \\ &\geq \frac{1}{4x} \left(\frac{1}{4} \int_{3/2}^{2x+1/2} \exp\left(-\frac{t^2}{8x}\right) dt + \frac{3}{4} \int_{1/2}^{2x-1/2} \exp\left(-\frac{t^2}{8x}\right) \left(1 - \frac{t^3}{78x^2}\right) dt \right) \\ &\geq \frac{1}{4x} \left(\frac{1}{4} \int_0^{2x} \exp\left(-\frac{t^2}{8x}\right) dt + \frac{3}{4} \int_0^{2x} \exp\left(-\frac{t^2}{8x}\right) \left(1 - \frac{t^3}{78x^2}\right) dt - \frac{9}{8} \right) \\ &\geq \frac{1}{4x} \left(\int_0^{2x} \exp\left(-\frac{t^2}{8x}\right) dt - \frac{3}{4} \int_0^{+\infty} \exp\left(-\frac{t^2}{8x}\right) \frac{t^3}{78x^2} dt - \frac{9}{8} \right) \\ &= \frac{1}{4x} \left(\int_0^{x/2} e^{-u} \frac{\sqrt{2x} du}{\sqrt{u}} - \frac{1}{104} \int_0^{+\infty} e^{-u} \frac{u du}{2} - \frac{9}{8} \right) \\ &\geq \frac{1}{4x} \left(\int_0^{+\infty} e^{-u} \frac{\sqrt{2x} du}{\sqrt{u}} - \frac{235}{208} - 2e^{-x/2} \right) > \frac{\sqrt{2\pi}}{4x^{1/2}} - \frac{0.586}{x}. \end{aligned}$$

All this finally yields the estimate

$$(55) \quad T'(x) - T''(x) = -\frac{5}{24} \frac{\sqrt{2\pi}}{x^{1/2}} + R_8(x), \quad -\frac{0.515}{x} < R_8(x) < \frac{1.303}{x}.$$

There only remains to evaluate $U'(x)$. According to (45), a change of variable $\ell = \ell' + 1$ followed by a decomposition $4x = (4x - \ell) + \ell$ allows us to transform the second summation

appearing in $U'(x)$ as

$$\begin{aligned} U'(x) &= \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)} \frac{(4x)^\ell}{4x \cdots (4x+\ell)} - \sum_{\ell=1}^{2x-2} \frac{1}{2\ell} \frac{4x(4x-1) \cdots (4x-\ell+1)}{(4x)^{\ell+1}} \\ &= \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)} \frac{(4x)^{\ell-1}}{(4x+1) \cdots (4x+\ell)} - \sum_{\ell=1}^{2x-2} \frac{1}{2\ell} \frac{(4x-1) \cdots (4x-\ell+1)(4x-\ell)}{(4x)^{\ell+1}} \\ &\quad - \sum_{\ell=1}^{2x-2} \frac{1}{2} \frac{(4x-1) \cdots (4x-\ell+1)}{(4x)^{\ell+1}}. \end{aligned}$$

Writing $\frac{1}{\ell+1} = \frac{1}{\ell} - \frac{1}{\ell(\ell+1)}$, one obtains

$$U'(x) = \frac{1}{4x} T'(x) - R_9(x)$$

with

$$\begin{aligned} R_9(x) &= \sum_{\ell=1}^{2x-1} \frac{1}{2\ell(\ell+1)} \frac{(4x)^{\ell-1}}{(4x+1) \cdots (4x+\ell)} + \sum_{\ell=1}^{2x-2} \frac{1}{2} \frac{(4x-1) \cdots (4x-\ell+1)}{(4x)^{\ell+1}} \\ &\quad - \left(\frac{1}{2\ell} \frac{(4x-1) \cdots (4x-\ell)}{(4x)^{\ell+1}} \right)_{\ell=2x-1}, \end{aligned}$$

and for $x \geq 2$, we find an upper bound

$$0 < R_9(x) < \frac{1}{4x} \sum_{\ell=1}^{+\infty} \frac{1}{2\ell(\ell+1)} + \frac{1}{2}(2x-2) \frac{1}{(4x)^2} < \frac{3}{16x}.$$

Thanks to an explicit calculation of $U'(x)$ for $x = 1, 2, 3$, we get the estimate

$$(56) \quad |U'(x)| < \frac{0.206}{x}.$$

Combining (25) (31'), (47), (48''), (49), (50) and (53-56), we now obtain

$$(57) \quad \Delta(x) = \frac{e^{-4x}}{4\pi x} \left(-\frac{5\sqrt{2\pi}}{12x^{1/2}} + R(x) \right)$$

with

$$R(x) = -U'(x) + \pi \left(R_1(x) + R_2(x) - R_3(x) \right) - \frac{5}{4} R_4(x) + 2 R_5(x) - R_6(x) + R_7(x) + 2 R_8(x),$$

whence

$$(58) \quad |R(x)| < \frac{10.835}{x}.$$

These estimates imply (12), (13). The proof of the Theorem is complete. \square

Numerical complexity of the Brent-McMillan algorithm for the calculation of Euler's constant. The refined version yields an error smaller than e^{-8x} . This implies to take $x = \frac{1}{8} d \log 10$ and leads to the time complexity

$$B'(d) = \left(\frac{3}{4}a_3 + \frac{1}{2}\right) \log 10 d^2 \simeq 9.7 d^2,$$

shorter than the time required by all other algorithms presented here.

We end up this discussion by giving the “hit-parade” of computation times of all those algorithms, arranged in order of increasing efficiency.

Algorithms	Euler		Sweeney						Brent-McM.	
	E_1	E_2	S_1	S_2	S'_1	S'_2	S_3	S'_3	B	B'
Computing time / d^2	$\frac{Cd}{(\log d)^2}$	$C \log d$	49.6	37.6	26.7	26.0	22.7	16.9	12.4	9.7

One should observe that there exist faster algorithms that compute γ up to d digits in less than $O(d(\log d)^3 \log \log d)$ units of time, at least theoretically. These are based on a use of the fast multiplication algorithm of Schönhage-Strassen [20], combined with a “block type” factorization of the relevant power series $F(x)$ (resp. $e^x, I_0(x), S_0(x)$) ; see Brent [6]. Such “fast algorithms” are however difficult to implement, and they outperform the “standard algorithms” presented here only when d is very large.

4. Continued fraction expansion of γ

The numerical value of γ obtained by the above mentioned authors has been used to determine the continued fraction expansion of γ and e^γ , which are now known up to 29 000 terms (Brent-McMillan [11]). The statistical distribution of the successive terms shows no significant deviation at a level of 5% from the Gauss-Kusmin distribution that expresses the frequency of a term equal to n in the expansion of a “random” real number (see Khintchine [16]):

$$f_n = \log_2 \left(1 + \frac{1}{n}\right) - \log_2 \left(1 + \frac{1}{n+1}\right).$$

In this way, one also obtains the following result which makes extremely unlikely that either γ or e^γ could be rational:

Theorem. — *If any of the numbers γ or e^γ is a rational number p/q with positive integers p and q , then $q > 10^{15\,000}$.*

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