Precise error estimate of the Brent-McMillan algorithm for the computation of Euler's constant

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Abstract. Brent and McMillan introduced in 1980 a new algorithm for the computation of Euler's constant γ, based on the use of the Bessel functions $I_0(x)$ and $K_0(x)$. It is the fastest known algorithm for the computation of γ. The time complexity can still be improved by evaluating a certain divergent asymptotic expansion up to its minimal term. Brent-McMillan conjectured in 1980 that the error is of the same magnitude as the last computed term, and Brent-Johansson partially proved it in 2015. They also gave some numerical evidence for a more precise estimate of the error term. We find here an explicit expression of that optimal estimate, along with a complete self-contained formal proof and an even more precise error bound.

Key-words. Euler's constant, Bessel functions, elliptic integral, integration by parts, asymptotic expansion, Euler-Maclaurin formula

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0. Introduction

Let $H_n = 1 + \frac{1}{2} + \cdots + \frac{1}{n}$ denote as usual the partial sums of the harmonic series. The algorithm introduced by Brent-McMillan [BM80] for the computation of Euler's constant $\gamma = \lim_{n\to+\infty}(H_n - \log n)$ is based on certain identities satisfied by the Bessel functions $I_\alpha(x)$ and $K_0(x)$:

$$(0.1) \qquad I_\alpha(x) = \sum_{n=0}^{+\infty} \frac{x^{\alpha+2n}}{n!\,\Gamma(\alpha+n+1)}, \qquad K_0(x) = -\frac{\partial I_\alpha(x)}{\partial \alpha}_{|\alpha=0}.$$

Experts will observe that $2x$ has been substituted to x in the conventional notation of Watson's treatise [Wat44]. A use of the formula $\Gamma'(n+1) = (H_n - \gamma)\,n!$, itself a consequence of the equalities $\frac{\Gamma'(x+1)}{\Gamma(x+1)} = \frac{1}{x} + \frac{\Gamma'(x)}{\Gamma(x)}$ and $\Gamma'(1) = -\gamma$, combined with a differentiation of I_α, yields the equalities

$$(0.2) \qquad K_0(x) = -(\log x + \gamma)I_0(x) + S_0(x) \qquad \text{where}$$

$$(0.3) \qquad I_0(x) = \sum_{n=0}^{+\infty} \frac{x^{2n}}{n!^2}, \qquad S_0(x) = \sum_{n=1}^{+\infty} H_n\,\frac{x^{2n}}{n!^2}.$$

Now, the Hankel integral formula (see [Art31]) 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 $x \to +\infty$:

$$I_0(x) = \frac{1}{\pi} \int_0^\pi e^{2x\cos u}\, du \qquad \text{hence} \quad I_0(x) \underset{x\to+\infty}{\sim} \frac{1}{\sqrt{4\pi x}}\, e^{2x}, \tag{0.4}$$

$$K_0(x) = \int_0^{+\infty} e^{-2x\cosh v}\, dv \qquad \text{hence} \quad K_0(x) \underset{x\to+\infty}{\sim} \sqrt{\frac{\pi}{4x}}\, e^{-2x}. \tag{0.5}$$

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

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

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 $\frac{1}{\sqrt{1-t/4x}} \geqslant 1 + t/8x$ and an integration by parts of the term $\sqrt{t}\, e^{-t}$, which give

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

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

$$\gamma = \frac{S_0(x)}{I_0(x)} - \log x - \frac{K_0(x)}{I_0(x)}, \tag{0.6}$$

with

$$0<\frac{K_0(x)}{I_0(x)}<\pi\,e^{-4x}\qquad\text{if } x\geqslant 1. \tag{0.7}$$

In the simpler version (BM) of the algorithm proposed by Brent-McMillan, the remainder term $\frac{K_0(x)}{I_0(x)}$ is neglected ; a precision 10^{-d} is then achieved for $x\simeq\frac{1}{4}\,(d\,\log 10+\log\pi)$, and the power series $I_0(x)$, $S_0(x)$ must be summed up to $n=\lceil a_1x\rceil$ approximately, where a_p is the unique positive root of the equation

$$a_p(\log a_p-1)=p. \tag{0.8}$$

The calculation of

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

requires 2 arithmetic operations for each term, and that of

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

requires 4 operations. The time complexity of the algorithm (BM) is thus

$$BM(d)=a_1\times\frac{1}{4}\,d\;\log 10\times 6\times d\simeq 12.4\,d^2. \tag{0.9}$$

As in Sweeney's more elementary method [Swe63], the remainder term $K_0(x)/I_0(x)$ can be evaluated by means of an asymptotic expansion. In fact

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

and a change of variables

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

gives

$$r=\frac{1}{2}(\cosh v-\cos u),\qquad |1-r\,e^{i\theta}|=\Big|\cos\Big(\frac{u+iv}{2}\Big)\Big|^2,$$
$$r\,dr\,d\theta=\Big|\sin\Big(\frac{u+iv}{2}\Big)\cos\Big(\frac{u+iv}{2}\Big)\Big|^2\,du\,dv=r\;|1-r\,e^{i\theta}|\,du\,dv,$$

therefore

$$I_0(x)K_0(x)=\frac{1}{2\pi}\int_0^{+\infty}\exp(-4xr)\;dr\int_0^{2\pi}\frac{d\theta}{|1-r\,e^{i\theta}|}. \tag{0.10}$$

Let us denote by

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

the (generalized) binomial coefficients. For $z = r\,e^{i\theta}$ and $|z| = r < 1$ the binomial identity $(1-z)^{-1/2} = \sum_{k=0}^{+\infty} \binom{-\frac12}{k} (-z)^k$ combined with the Parseval-Bessel formula yields the expansion

$$\varphi(r) := \frac{1}{2\pi}\int_0^{2\pi} \frac{d\theta}{|1 - r\,e^{i\theta}|} = \sum_{k=0}^{+\infty} w_k\, r^{2k} \qquad \text{for } 0 \leqslant r < 1, \tag{0.11}$$

where the coefficient

$$w_k := \binom{-1/2}{k}^2 = \left(\frac{1\cdot 3\cdot 5\cdots(2k-1)}{2\cdot 4\cdot 6\cdots 2k}\right)^2 = \frac{(2k)!^2}{2^{4k}\,k!^4}. \tag{0.12}$$

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

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

whence $w_k = (\frac{2}{\pi} W_{2k})^2$. 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 $\sqrt{\frac{\pi}{2(2k+1)}} < W_{2k} < \sqrt{\frac{\pi}{4k}}$, therefore

$$\frac{2}{\pi(2k+1)} < w_k < \frac{1}{\pi k}. \tag{0.13}$$

The main new ingredient of our analysis for estimating $I_0(x)K_0(x)$ is the following integral formula derived from (0.10), (0.11) :

$$I_0(x)K_0(x) = \int_0^{+\infty} e^{-4xr}\,\varphi(r)\,dr \tag{0.14}$$

where

$$\varphi(r) = \sum_{k=0}^{+\infty} w_k\, r^{2k} \qquad \text{for } r < 1, \tag{0.15}$$

$$\varphi(r) = \frac{1}{r}\varphi\left(\frac{1}{r}\right) = \sum_{k=0}^{+\infty} w_k\, r^{-2k-1} \qquad \text{for } r > 1. \tag{0.16}$$

(The last identity can be seen immediately by applying the change of variable $\theta \mapsto -\theta$ in (0.11)). It is also easily checked using (0.13) that one has an equivalent

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

in particular the integral (0.14) converges near $r = 1$ (later, we will need a more precise approximation, but more sophisticated arguments are required for this). 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 $r \geqslant 1$, one formally obtains a divergent asymptotic expansion

$$I_0(x)K_0(x) \sim \sum_{k\in\mathbb{N}} w_k\,\frac{(2k)!}{(4x)^{2k+1}} \sim \frac{1}{4x}\sum_{k\in\mathbb{N}} \frac{(2k)!^3}{k!^4\,(16x)^{2k}}. \tag{0.17}$$

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

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

The idea is to truncate the asymptotic expansion precisely at $k = 2x$. We will check, as was conjectured by Brent-McMillan [BM80] and partly proven by Brent and Johansson [BJ15] 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 Stirling's formula.

Theorem. *The truncation error*

$$\Delta(x) := I_0(x)K_0(x) - \frac{1}{4x}\sum_{k=0}^{2x}\frac{(2k)!^3}{k!^4\,(16x)^{2k}} \tag{0.18}$$

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

$$\Delta(x) \sim -\frac{5\,e^{-4x}}{24\sqrt{2\pi}\,x^{3/2}}, \tag{0.19}$$

and more specifically

$$\Delta(x) = -e^{-4x}\left(\frac{5}{24\sqrt{2\pi}\,x^{3/2}} + \varepsilon(x)\right), \qquad |\varepsilon(x)| < \frac{0.863}{x^2}. \tag{0.20}$$

The approximate value

$$\frac{K_0(x)}{I_0(x)} \simeq \frac{1}{4x\,I_0(x)^2}\sum_{k=0}^{2x}\frac{(2k)!^3}{k!^4\,(16x)^{2k}} \tag{0.21}$$

is thus affected by an error of magnitude

$$\frac{\Delta(x)}{I_0(x)^2} \sim -\frac{5\sqrt{2\pi}}{12\,x^{1/2}}\,e^{-8x}. \tag{0.22}$$

The refined version (BM') of the Brent-McMillan algorithm consists in evaluating the remainder term $\frac{K_0(x)}{I_0(x)}$ up to the accuracy e^{-8x} permitted by the approximation (0.22). This implies to take $x = \frac{1}{8}\,d\log 10$ and leads to a time complexity

$$BM'(d) = \left(\frac{3}{4}a_3 + \frac{1}{2}\right)\log 10\; d^2 \simeq 9.7\,d^2, \tag{0.23}$$

substantially better than (0.9). The proof of the above theorem requires many calculations. The techniques developed here would probably even yield an asymptotic development for $\Delta(x)$, at least for the first few terms, but the required calculations seem very extensive. Hopefully, further asymptotic expansions of the error might be useful to investigate the arithmetic properties of γ, especially its rationality or irrationality.

The present paper is an extended version of an original text [Dem85] written in June 1984 and published in "Gazette des Mathématiciens" in 1985. However, because of length constraints for such a mainstream publication, the main idea for obtaining the error estimate of the Brent-McMillan algorithm had only been hinted, and most of the details had been omitted. After more than 30 years passed, we take the opportunity to make these details available and to improve the recent results of Brent-Johansson [BJ15].

1. Expression of the error in terms of elliptic integrals

By (0.10) and the definition of $\Delta(x)$ we have

$$\Delta(x) = \int_0^{+\infty} e^{-4xr}\,\delta(r)\,dr \tag{1.1}$$

where

$$\delta(r) := \varphi(r) - \sum_{k=0}^{2x} w_k\, r^{2k}, \qquad \text{so that} \quad \delta(r) = \sum_{k=2x+1}^{+\infty} w_k\, r^{2k} \quad \text{for} \quad r < 1. \tag{1.2}$$

For $r < 1$, let us also 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 $r \to 1$. 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

$$\begin{aligned}\varphi(r) &= \frac{2}{\pi}\int_0^{\pi/2}(1-r^2\cos^2\theta)^{-1/2}\,d\theta = \frac{2}{\pi}\int_0^{+\infty}\frac{du}{\sqrt{(1+u^2)(t^2+u^2)}}\,du\\ &= \frac{4}{\pi}\int_0^1 \frac{dv}{\sqrt{(1+v^2)(1+t^2v^2)}} + \frac{2}{\pi}\int_t^1\frac{dv}{\sqrt{(1+v^2)(t^2+v^2)}} \qquad (1.3)\end{aligned}$$

where the last line is obtained by splitting the integral $\int_0^{+\infty}\ldots du$ 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 (1.3) admits a development as a convergent series

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

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

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

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

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

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)

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

In fact, we see a priori from (0.13) that

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

and

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

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

$$\varphi(r)=\frac{1}{\pi}\left(\varphi(t)\,\log\frac{1}{t^2}+4\sum_{k=0}^{+\infty}c_k\,t^{2k}\right),\qquad c_k=c'_k+c''_k,\tag{1.4}$$

and this identity will produce an arbitrarily precise expansion of $\varphi(r)$ when $r\to 1$. 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

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

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

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

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

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

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

$$c_k = w_k\left(\log 2 - \sum_{\ell=1}^{2k}\frac{(-1)^{\ell-1}}{\ell}\right). \tag{1.5}$$

The remainder of the alternating series expressing $\log 2$ is bounded by half of last calculated term, namely $1/4k$, thus according to (0.13) we have $0 < c_k < \frac{1}{\pi^2 k^2}$ if $k \geqslant 1$, and the radius of convergence of the series is is 1. From (0.14) and (1.4) we infer as $r \to 1-0$ the well known expansion of the elliptic integral

$$\varphi(r) = \frac{1}{\pi}\left(\sum_{k=0}^{+\infty} w_k t^{2k} \log\frac{1}{t^2} + 4\sum_{k=0}^{+\infty} c_k t^{2k}\right), \qquad t^2 = 1 - r^2, \tag{1.6}$$

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 $r = 1+h$, $h \to 0$. 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

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

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

$$\begin{aligned}
\varphi(1+h) = \frac{1}{\pi}\Bigg(&\log\frac{1}{|h|} + 3\log 2 - \frac{1}{2}h\log\frac{1}{|h|} - \left(\frac{3}{2}\log 2 - \frac{1}{2}\right)h\\
&+ \frac{5}{16}h^2\log\frac{1}{|h|} + \left(\frac{15}{16}\log 2 - \frac{7}{16}\right)h^2 + O\left(h^3\log\frac{1}{|h|}\right)\Bigg).
\end{aligned} \tag{1.7}$$

For $r = 1+h > 1$, the identity $\varphi(r) = \frac{1}{r}\varphi(\frac{1}{r})$ 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 (1.7) is still valid for $h > 0$. Passing to the limit $r \to 0$, $t \to 1-0$ in (1.6) implies the relation $\sum_{k\geqslant 0} c_k = \frac{\pi}{4}$. The following Lemma will be useful.

Lemma A. *For $h > 0$, the difference*

$$\rho(h) = \varphi(1+h) - \frac{1}{\pi}\left(\log\frac{1}{h} + 3\log 2 - \frac{1}{2}h\,\log\frac{1}{h} - \left(\frac{3}{2}\log 2 - \frac{1}{2}\right)h\right) \tag{1.8}$$

$$= \varphi(1+h) - \frac{1}{2\pi}\left((h-2)\log\frac{h}{8} + h\right) \tag{1.9}$$

admits the upper bound

$$|\rho(h)| \leqslant h^2\left(2 + \log\left(1 + \frac{1}{h}\right)\right). \tag{1.10}$$

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 $t^2 \leqslant 2h$ and

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

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

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

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

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

with $\theta_i \in \,]0,1[$. In order to estimate $\rho(h)$, we we fully expand this expression and replace each term by an upper bound of its absolute value. For $h \leqslant \frac{1}{4}$, this shows that $|\rho(h)| \leqslant h^2(0.885\,\log\frac{1}{h} + 2.11)$, so that (1.10) is satisfied. For $h \geqslant \frac{1}{4}$, we write

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

and by (0.13) 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

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

This implies

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

therefore $|\rho'(h)|\leqslant\frac{1}{2\pi}(h-1-\log 8+2)\leqslant\frac{1}{2\pi}h$ for $h\in[2,+\infty[$. Since $\rho(2)\simeq 0.00249<\frac{1}{\pi}$, we see that $|\rho(h)|\leqslant\frac{1}{4\pi}h^2$, and this shows that (1.10) still holds on $[2,+\infty[$. A numerical calculation of $\rho(h)$ at sufficiently close points in the interval $[\frac{1}{4},2]$ finally yields (1.10) on that interval. □

Now we split the integral (1.1) 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

$$\int_1^{+\infty}e^{-4xr}\,\varphi(r)\,dr=\frac{e^{-4x}}{4x}\int_0^{+\infty}e^{-t}\,\varphi\Big(1+\frac{t}{4x}\Big)\,dt,\tag{1.11}$$

and Lemma A (1.9) yields for this integral an approximation

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

with an error bounded by

$$\begin{aligned}&\frac{e^{-4x}}{4x}\int_0^{+\infty}e^{-t}\Big(\frac{t}{4x}\Big)^2\bigg(2+\log\Big(1+\frac{4x}{t}\Big)\bigg)dt\\&\qquad\qquad=\frac{e^{-4x}}{4x}\bigg(\frac{1}{4x^2}+\frac{1}{16x^2}\int_0^{+\infty}t^2\,e^{-t}\,\log\frac{t+4x}{t}\,dt\bigg).\end{aligned}$$

Writing

$$0<\log\frac{t+4x}{t}=\log\frac{4x}{t}+\log\Big(1+\frac{t}{4x}\Big)\leqslant\log\frac{4x}{t}+\frac{t}{4x},$$

we further see that

$$\int_0^{+\infty}t^2\,e^{-t}\,\log\frac{t+4x}{t}\,dt\leqslant\int_0^{+\infty}t^2\,e^{-t}\,\Big(\log\frac{4x}{t}+\frac{t}{4x}\Big)\,dt=2\log 4x+\frac{3}{2x}+2\gamma-3.$$

We infer

$$\int_1^{+\infty} e^{-4xr}\,\varphi(r)\,dr = \frac{e^{-4x}}{4\pi x}\Big(\log x + \gamma + 5\log 2 - \frac{\log x}{8x}\Big) + \frac{e^{-4x}}{4x}\,R_1(x), \tag{1.12}$$

with

$$|R_1(x)| < \frac{\gamma + 5\log 2 - 2}{8\pi x} + \frac{1}{4x^2} + \frac{2\log 4x + \frac{3}{2x} + 2}{16x^2} < \frac{0.483}{x} \quad \text{if } \mathbb{N} \ni x \geqslant 1, \tag{1.13}$$

thanks to a numerical evaluation of the sequence in a suitable range.

2. Estimate of the truncated asymptotic expansion

We now estimate the two integrals $\int_0^1 e^{-4xr} \sum\limits_{k\geqslant 2x+1} w_k\, r^{2k}\, dr$, $\int_1^{+\infty} e^{-4xr} \sum\limits_{k\leqslant 2x} w_k\, r^{2k}\, dr$. By means of iterated integrations by parts, we get

$$\int_0^1 e^{-4xr}\, r^{2k}\, dr = e^{-4x} \sum_{\ell=1}^{+\infty} \frac{(4x)^{\ell-1}}{(2k+1)\cdots(2k+\ell)}, \tag{2.1}$$

$$\int_1^{+\infty} e^{-4xr}\, r^{2k}\, dr = \frac{e^{-4x}}{4x}\Big(1 + \sum_{\ell=1}^{2k} \frac{2k(2k-1)\cdots(2k-\ell+1)}{(4x)^\ell}\Big). \tag{2.2}$$

Combining the identities (1.1), (1.2), (1.12), (2.1), (2.2) we find

$$\Delta(x) = \frac{e^{-4x}}{4x}\bigg(\frac{1}{\pi}\Big(\log x + \gamma + 5\log 2\Big) - \frac{\log x}{8\pi x} - \sum_{k=0}^{2x} w_k + S(x) + R_1(x) + R_2(x)\bigg) \tag{2.3}$$

with

$$S(x) = \sum_{k=2x+1}^{+\infty} \sum_{\ell=1}^{2x-1} \frac{w_k\,(4x)^\ell}{(2k+1)\cdots(2k+\ell)} - \sum_{k=1}^{2x} \sum_{\ell=1}^{2x-1} w_k\, \frac{2k(2k-1)\cdots(2k-\ell+1)}{(4x)^\ell}, \tag{2.4}$$

and

$$R_2(x) = \sum_{k=2x+1}^{+\infty} \sum_{\ell=2x}^{+\infty} \frac{w_k\,(4x)^\ell}{(2k+1)\cdots(2k+\ell)} - \sum_{k=1}^{2x} \sum_{\ell=2x}^{+\infty} w_k\, \frac{2k(2k-1)\cdots(2k-\ell+1)}{(4x)^\ell} \tag{2.5}$$

(In the final summation, terms of index $\ell > 2k$ are zero). Formula (2.3) leads us to study the asymptotic expansion of $\sum_{k=0}^{2x} w_k$. This development is easy to establish from (1.6) (one could even calculate it at an arbitrarily large order).

Lemma B. *One has*

$$w_k = \frac{1}{\pi k}\Big(1 - \frac{1}{2(2k-1)} + \varepsilon_k\Big) \quad \textit{where} \quad \frac{1}{12k(2k-1)} < \varepsilon_k < \frac{5}{16k(2k-1)}, \quad k \geqslant 1, \tag{2.6}$$

$$\sum_{k=0}^{2x} w_k = \frac{1}{\pi}\Big(\log x + 5\log 2 + \gamma\Big) + R_3(x), \qquad \frac{1}{4\pi x} < R_3(x) < \frac{19}{48\pi x}. \tag{2.7}$$

Proof. The lower bound (2.6) is a consequence of the Euler-Maclaurin's formula [Eul15] 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

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

The inequality $e^{-x} \geqslant 1-x$ 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 (2.6) follows for all $k \geqslant 1$. 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 $e^{-x} \leqslant 1 - x + \frac{1}{2}x^2$ 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)

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

One can check that the final inequality still holds for $k = 1, 2$, and this implies the estimate (2.6). On the other hand, formula (1.6) yields

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

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

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

We infer

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

and the upper and lower bounds in (2.6) imply

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

The Euler-Maclaurin estimate

$$\sum_{k=1}^{2x} \frac{1}{k} = \log(2x) + \gamma + \frac{1}{4x} + \frac{b_2}{2(2x)^2} - \frac{b_4}{4(2x)^4} + \cdots \tag{2.8}$$

then finally yields (2.7). □

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 (2.6) obtained in Lemma B implies

$$S(x) = \frac{2}{\pi} \Big(T(x) - \frac{1}{2} U(x) + \frac{5}{8} R_4(x)\Big), \tag{2.9}$$

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

$$T(x) = \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell}{2k(2k+1)\cdots(2k+\ell)} - \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-1)\cdots(2k-\ell+1)}{(4x)^\ell}, \tag{2.10}$$

$$U(x) = \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell}{(2k-1)\cdots(2k+\ell)} - \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-2)\cdots(2k-\ell+1)}{(4x)^\ell}, \tag{2.11}$$

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

$$|R_4(x)| \leqslant \sum_{\ell=1}^{2x-1} \sum_{k=2x+1}^{+\infty} \frac{(4x)^\ell/2k}{(2k-1)\cdots(2k+\ell)} + \sum_{\ell=1}^{2x-1} \sum_{k=1}^{2x} \frac{(2k-2)\cdots(2k-\ell+1)}{2k\,(4x)^\ell}. \tag{2.12}$$

3. Application of discrete integration by parts

To evaluate the sums $T(x)$, $U(x)$ and $R_4(x)$, our method consists in performing first a summation over the index k, and for this, we use "discrete integrations by parts". Set

$$u_k^{a,b} := \frac{1}{(2k+a)(2k+a+1)\cdots(2k+b-1)}, \qquad a \leqslant b \tag{3.1}$$

(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 $2(2k+a) \leqslant 4k+a+b+1 \leqslant 2(2k+b+1)$ imply

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

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

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

with an upward error equal to

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

and an "error on the error" (again upwards) equal to

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

In other words, we find

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

$$(3.2_3^{a,b})\qquad +\theta\,\frac{b-a+1}{8}\,\frac{1}{(4x+a-1)\cdots(4x+b)},\qquad \theta\in[0,1].$$

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 $(3.2_p^{a,b})$, and will use it here in the cases $p=2,3$. For the summations $\sum_{k=1}^{2x}\dots$, we similarly define

$$(3.3)\qquad v_k^{a,b}=(2k-a)(2k-a-1)\cdots(2k-b+1),\qquad a\leqslant b,$$

and obtain

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

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

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

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

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

with a downward error

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

and an upward error on the error equal to

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

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

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

$$(3.4_3^{a,b})\qquad =\frac{1}{2(b-a)}\,v_{2x}^{a,b}+\frac{1}{4}\,v_{2x}^{a,b-1}-\theta\,\frac{b-a-1}{8}\,v_{2x}^{a,b-2}+C_3^{a,b},$$

with

$$(3.5_3^{a,b})\qquad |C_3^{a,b}|\leqslant \frac{1}{2(b-a)}|v_0^{a,b}|+\frac14|v_0^{a,b-1}|+\frac{b-a-1}{8}|v_0^{a,b-2}|,$$

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

$$\sum_{k=1}^{2x}(2k-a-2)\cdots(2k-b)=\frac{1}{2(b-a)}\Big(v_{2x}^{a,b}-v_0^{a,b}\Big)-\theta\,\frac14\Big(v_{2x}^{a,b-1}-v_0^{a,b-1}\Big)$$

$$(3.6_2^{a,b})\qquad =\frac{1}{2(b-a)}\,(4x-a)\cdots(4x-b+1)-\theta\,\frac14\,(4x-a)\cdots(4x-b+2)+C_2^{a,b}.$$

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

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

If we apply this equality to the values (a,b), $(a,b-1)$ and $k=2x$, we see that the $(3.4_3^{a,b})$ development can be written in the equivalent form

$$\begin{aligned}&\sum_{k=1}^{2x}(2k-a-1)\cdots(2k-b+1)-C_3^{a,b}\\&=\frac{1}{2(b-a)}v_{2x}^{a+1,b+1}+\frac34 v_{2x}^{a+1,b}+\frac{b-a-1}{8}\Big(2\,v_{2x}^{a+1,b-1}-\theta\,v_{2x}^{a,b-2}\Big),\\&=\frac{1}{2(b-a)}\,(4x-a-1)\cdots(4x-b)+\frac34\,(4x-a-1)\cdots(4x-b+1)\end{aligned}$$

$$(3.7_3^{a,b})\qquad +\frac{b-a-1}{8}\Big(2(4x-a-1)\cdots(4x-b+2)-\theta\,(4x-a)\cdots(4x-b+3)\Big)$$

According to (2.10), $(3.2_3^{0,\ell})$ and $(3.7_3^{0,\ell})$, we get

$$(3.8)\qquad T(x)=T'(x)-T''(x)+R_5(x)$$

with

$$(3.9)\qquad T'(x)=\sum_{\ell=1}^{2x-1}\frac{1}{2\ell}\bigg(\frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)}-\frac{(4x-1)\cdots(4x-\ell)}{(4x)^\ell}\bigg),$$

$$(3.10)\qquad T''(x)=\sum_{\ell=1}^{2x-1}\frac14\,\frac{(4x)^\ell}{4x(4x+1)\cdots(4x+\ell)}+\frac34\,\frac{(4x-1)\cdots(4x-\ell+1)}{(4x)^\ell},$$

$$(3.11)\qquad |R_5(x)|\leqslant\frac18\sum_{\ell=1}^{2x-1}\bigg(\frac{(\ell+1)\,(4x)^\ell}{(4x-1)4x\cdots(4x+\ell)}+\frac{2(\ell-1)\,(4x-1)\cdots(4x-\ell+2)}{(4x)^\ell}\bigg).$$

The last term in the last line comes from formula $(3.7_3^{0,\ell})$, by observing that the inequalities $4x\leqslant 2(4x-\ell+2)$ $\ell\leqslant 2x-1$ imply

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

Similarly, thanks to (2.11), $(3.2_2^{-1,\ell})$ and $(3.6_2^{0,\ell-1})$, we obtain the decomposition

$$U(x)=U'(x)-U''(x)+R_6(x) \tag{3.12}$$

with

$$U'(x)=\sum_{\ell=1}^{2x-1}\frac{1}{2(\ell+1)}\,\frac{(4x)^\ell}{4x\cdots(4x+\ell)}-\sum_{\ell=2}^{2x-1}\frac{1}{2(\ell-1)}\,\frac{4x(4x-1)\cdots(4x-\ell+2)}{(4x)^\ell}, \tag{3.13}$$

$$U''(x)=\frac{1}{4x}\sum_{k=1}^{2x}\frac{1}{2k-1}\qquad\text{(negative term } \ell=1 \text{ appearing in } U(x)\text{)}, \tag{3.14}$$

$$|R_6(x)|\leqslant\frac14\sum_{\ell=1}^{2x-1}\frac{(4x)^\ell}{(4x-1)\cdots(4x+\ell)}+\frac14\sum_{\ell=2}^{2x-1}\frac{4x(4x-1)\cdots(4x-\ell+3)}{(4x)^\ell}. \tag{3.15}$$

The remainder terms $R_2(x)$ [resp. $R_4(x)$] can be bounded in the same way by means of $(3.2_2^{0,\ell})$ and $(3.6_2^{-1,\ell-1})$ [resp. $(3.2_2^{-1,\ell})$ and $(3.6_2^{0,\ell-2})$] and (0.13), (2.5), (2.12) lead to

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

$$\leqslant\frac{2}{\pi}\sum_{\ell=2x}^{+\infty}\frac{1}{2\ell}\left(\frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)}+\frac{(4x+1)\cdots(4x-\ell+2)}{(4x)^\ell}\right), \tag{3.16}$$

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

$$\leqslant\sum_{\ell=1}^{2x-1}\frac{1}{2(\ell+1)}\,\frac{(4x)^{\ell-1}}{4x\cdots(4x+\ell)}+\sum_{\ell=3}^{2x-1}\frac{1}{2(\ell-2)}\,\frac{4x(4x-1)\cdots(4x-\ell+3)}{(4x)^\ell} \tag{3.17}$$

$$+\sum_{k=1}^{2x}\frac{1}{2k(2k-1)}\,\frac{1}{4x}+\sum_{k=1}^{2x}\frac{1}{(2k-1)}\,\frac{1}{(4x)^2}\quad\text{[terms } \ell=1,2 \text{ in the summation]}. \tag{3.18}$$

Finally, by (2.3), (2.7), (2.9) and (3.8), (3.12) we get the decomposition

$$\Delta(x)=\frac{e^{-4x}}{4\pi x}\Bigg(2\,T'(x)-2\,T''(x)-U'(x)+U''(x)-\frac{\log x}{8x}$$

$$+\,\pi\Big(R_1(x)+R_2(x)-R_3(x)\Big)-\frac54 R_4(x)+2\,R_5(x)-R_6(x)\Bigg). \tag{3.19}$$

Lemma C. *The following inequalities hold*:

$$\log 2-\frac{1}{8x}<\sum_{k=1}^{2x}\frac{1}{2k(2k-1)}<\log 2-\frac{1}{2(4x+1)}, \tag{3.20}$$

$$\sum_{k=1}^{2x}\frac{1}{2k-1}<\frac32\log 2+\frac12\Big(\log x+\gamma\Big)+\frac{1}{24x^2}, \tag{3.21}$$

$$U''(x)=\frac{\log x}{8x}+R_7(x),\qquad 0<R_7(x)<\frac{1.37}{x}. \tag{3.22}$$

Proof. To check (3.20), we observe that the sum of the series is $\log 2$ and that the remainder of index $2x$ admits the lower and upper bounds

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

According to the Euler-Maclaurin expansion (2.8), we get on the one hand

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

whence (3.21), and on the other hand

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

A straightforward numerical computation gives $\frac{3}{2}\log 2 + \frac{1}{2}\gamma + \frac{1}{24} < 1.37$, which then yields (3.22). $\square$

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

$$(3.23)\quad |R_6(x)| \leqslant \frac{1}{4}\sum_{\ell=1}^{2x-1} \frac{1}{4x(4x-1)} + \frac{1}{4}\sum_{\ell=2}^{2x-1} \frac{1}{(4x)^2} \leqslant \frac{1}{4}\,\frac{2x-1}{4x(4x-1)} + \frac{1}{4}\,\frac{2x-2}{(4x)^2} < \frac{1}{16x}.$$

Consider now $R_4(x)$. We use Lemma C to bound both summations appearing in (3.18), and get in this way

$$[[(3.18)]] \leqslant \frac{\log 2 - \frac{1}{2(4x+1)}}{4x} + \frac{\frac{3}{2}\log 2 + \frac{1}{2}(\log x + \gamma) + \frac{1}{24x^2}}{(4x)^2} < \frac{0.234}{x}$$

(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

$$\sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)}\,\frac{(4x)^{\ell-1}}{4x\cdots(4x+\ell)} \leqslant \sum_{\ell=1}^{2x-1} \frac{1}{2(\ell+1)}\,\frac{1}{(4x)^2} \leqslant \frac{\log 2x+\gamma+\frac{1}{4x}+\frac{1}{12(2x)^2}-1}{32x^2} < \frac{0.025}{x},$$

$$\sum_{\ell=3}^{2x-1} \frac{1}{2(\ell-2)}\,\frac{4x(4x-1)\cdots(4x-\ell+1)}{(4x)^{\ell+2}} \leqslant \sum_{\ell=1}^{2x-3} \frac{1}{\ell}\,\frac{1}{32x^2} \leqslant \frac{\log 2x+\gamma}{32x^2} < \frac{0.040}{x}.$$

This gives the final estimate

$$|R_4(x)| \leqslant \frac{0.299}{x}. \tag{3.24}$$

4. Further integral estimates

In order to get an optimal bound of the other terms, and especially their differences, we are going to replace some summations by suitable integrals. Before, we must estimate more precisely the partial products $\prod(4x \pm j)$, and for this, we use the power series expansion of their logarithms. For $t > 0$, we have $t - \frac{1}{2}t^2 < \log(1+t) < t$. By taking $t = \frac{j}{4x}$, we find

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

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

$$\exp\left(\frac{1}{32x} - \frac{(\ell+1/2)^2}{8x}\right) < \frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} < \exp\left(\frac{1}{32x} - \frac{(\ell+1/2)^2}{8x} + \frac{(\ell+1/2)^3}{96x^2}\right). \tag{4.1}$$

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

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

hence (after performing a suitable numerical calculation)

$$\begin{aligned} &\frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} < \exp\left(\frac{1}{32x} - \frac{5}{6}\,\frac{(\ell+1/2)^2}{8x}\right) && \text{for } \ell \leqslant 2x-1, \\ &\frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} < \exp\left(\frac{1}{32x} - \frac{5}{6}\,\frac{(2x-1/2)^2}{12x}\right) < \frac{1.52}{x} && \text{for } \ell \geqslant 2x-1. \end{aligned} \tag{4.2}$$

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

$$\sum_{\ell=2x}^{+\infty} \frac{(4x)^\ell}{(4x+1)\cdots(4x+\ell)} < \frac{1.52}{x}\sum_{p=1}^{+\infty}\left(\frac{2}{3}\right)^p < \frac{3.04}{x}. \tag{4.3}$$

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

$$-\frac{\ell(\ell+1)}{8x} - \frac{16\,\ell(\ell+1)(2\ell+1)}{6\cdot 26\,(4x)^2} < \log\frac{(4x-1)\cdots(4x-\ell)}{(4x)^\ell} < -\frac{\ell(\ell+1)}{8x}. \tag{4.4}$$

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

$$\frac{(4x+1)\cdots(4x-\ell+2)}{(4x)^\ell} \leqslant \Big(1+\frac{1}{4x}\Big)\exp\Big(-\frac{(\ell-1)(\ell-2)}{8x}\Big) < \exp\Big(-\frac{\ell(\ell-3)}{8x}\Big), \tag{4.5}$$

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

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

As $2\ell \geqslant 4x$, we deduce from (3.16) that

$$|R_2(x)| \leqslant \frac{2}{\pi}\,\frac{1}{4x}\,\frac{7.69}{x} < \frac{1.224}{x^2} \tag{4.6}$$

(but actually, one can see that $R_2(x)$ even decays exponentially). By means of a standard integral-series comparison, the inequalities (3.11), (4.2) and (4.4) also provide

$$\begin{aligned} |R_5(x)| &\leqslant \frac{1}{8}\sum_{\ell=1}^{2x-1} \frac{\ell+1}{4x(4x-1)} \exp\Big(\frac{1}{32x}-\frac{5}{6}\,\frac{(\ell+1/2)^2}{8x}\Big) + 2\,\frac{\ell-1}{(4x)^2}\exp\Big(\frac{3\ell}{8x}-\frac{\ell^2}{8x}\Big)\\ &\leqslant \frac{1}{8(4x)(3x)}\bigg(e^{\frac{1}{32}}\int_0^{+\infty}\Big(t+\frac{3}{2}\Big)\exp\Big(-\frac{5}{6}\,\frac{t^2}{8x}\Big)dt + \frac{3\,e^{\frac{3}{4}}}{2}\int_0^{+\infty} t\,\exp\Big(-\frac{t^2}{8x}\Big)dt\bigg)\\ &= \frac{1}{96x^2}\bigg(e^{\frac{1}{32}}\Big(\frac{24}{5}x+\frac{3}{2}\sqrt{\frac{48x}{5}}\,\frac{1}{2}\sqrt{\pi}\Big)+6\,e^{\frac{3}{4}}\,x\bigg) < \frac{0.229}{x} \qquad \text{for } x \geqslant 1. \end{aligned} \tag{4.7}$$

It then follows from (3.9) and (4.1) that

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

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

$\prod(1-a_j)^{-1}-1 \geqslant \sum a_j$, thus (4.3) implies

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

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

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

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

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

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

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

therefore

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

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

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

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

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

All other terms appearing in the integral involve terms $O(\frac{1}{x})$ with coefficients which are products of factors $\Gamma(a)$, $\frac{1}{2} \leqslant a \leqslant 2$, 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 $\Gamma(a) \leqslant \sqrt{\pi}$, we obtain

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

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

$$\begin{aligned}
T'(x) &\geqslant \sum_{\ell=1}^{2x-1} \exp\left(-\frac{(\ell+1/2)^2}{8x}\right)\left(1-\frac{(\ell+1/2)^3}{78\,x^2}\right)\frac{(\ell+1)(\ell+1/2)}{96x^2}\\
&\geqslant \int_{3/2}^{2x+1/2} \exp\left(-\frac{t^2}{8x}\right)\left(1-\frac{t^3}{78\,x^2}\right)\frac{(t-1)(t-1/2)}{96x^2}\,dt\\
&\geqslant \int_{2}^{2x} \exp\left(-\frac{t^2}{8x}\right)\left(1-\frac{t^3}{78\,x^2}\right)\frac{t^2-3t/2}{96x^2}\,dt\\
&= \int_{1/2x}^{x/2} e^{-u}\left(1-\frac{8\sqrt{8}\,u^{3/2}}{78\,x^{1/2}}\right)\frac{8xu-3\sqrt{8}\,x^{1/2}u^{1/2}/2}{96x^2}\,\frac{\sqrt{8}\,x^{1/2}\,du}{2\,u^{1/2}}\\
&\geqslant \int_{1/2x}^{x/2} e^{-u}\left(1-\frac{8\sqrt{8}\,u^{3/2}}{78\,x^{1/2}}\right)\frac{\sqrt{8}\,u-3\,x^{-1/2}u^{1/2}/2}{24\,x^{1/2}}\,\frac{du}{u^{1/2}}\\
&\geqslant \int_{1/2x}^{x/2} e^{-u}\left(\frac{\sqrt{2}\,u^{1/2}}{12\,x^{1/2}}-\frac{8\,u^2}{3\cdot 78\,x}-\frac{1}{16x}\right)du\\
&\geqslant \int_{0}^{+\infty} e^{-u}\left(\frac{\sqrt{2}\,u^{1/2}}{12\,x^{1/2}}-\frac{4\,u^2}{117\,x}-\frac{1}{16x}\right)du - \int_{\complement} e^{-u}\frac{\sqrt{2}\,u^{1/2}}{12\,x^{1/2}}\,du.
\end{aligned}$$

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

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

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

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

This provides an estimate

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

Therefore, we obtain the explicit lower bound

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

In the same manner, but now without any compensation of terms and with much simpler calculations, the estimates (3.11), (4.1), (4.3) provide an upper bound

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

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

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

and we get likewise a lower bound

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

All this finally yields the estimate

$$\text{(4.8)}\qquad T'(x)-T''(x)=-\frac{5}{24}\,\frac{\sqrt{2\pi}}{x^{1/2}}+R_8(x),\qquad -\frac{0.515}{x}<R_8(x)<\frac{1.303}{x}.$$

There only remains to evaluate $U'(x)$. According to (3.13), 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

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

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

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

and for $x \geqslant 2$, 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

$$|U'(x)| < \frac{0.206}{x}. \tag{4.9}$$

Combining (1.13), (2.7), (3.19), (3.22), (3.23), (3.24) and (4.6 – 4.9), we now obtain

$$\Delta(x) = \frac{e^{-4x}}{4\pi x}\left(-\frac{5\sqrt{2\pi}}{12\,x^{1/2}} + R(x)\right) \tag{4.10}$$

with

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

whence

$$|R(x)| < \frac{10.835}{x}. \tag{4.11}$$

These estimates imply (0.19 – 0.22). The proof of the Theorem is complete. □

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