

# SHORT MOLLIFIERS OF THE RIEMANN ZETA-FUNCTION

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**ABSTRACT.** We apply the calculus of variations to construct a new sequence of linear combinations of derivatives of the Riemann  $\zeta$ -function adapted to Levinson’s method, which yield a positive proportion of zeros of the  $\zeta$ -function on the critical line, regardless of how short the mollifier is. Our construction extends readily to modular  $L$ -functions. Even with Levinson’s original choice of mollifier, our method more than doubles the proportions of zeros on the critical line for modular  $L$ -functions previously obtained by Bernard and Kühn–Robles–Zeindler, while relying on the same arithmetic inputs. This indicates that optimizing the linear combinations, an approach that has received relatively little attention, has a more pronounced effect than refining the mollifier when it is short. Curiously, our linear combinations provide non-trivial smooth approximations of Siegel’s  $\mathfrak{f}$ -function in the celebrated Riemann–Siegel formula.

## 1. INTRODUCTION

There are two well-known methods for proving that a positive proportion of the zeros of the Riemann zeta-function  $\zeta(s)$  ( $s = \sigma + it$ ) lie on the critical line  $\sigma = 1/2$ : Selberg’s method [Sel42] and Levinson’s method [Lev74]. Both of these methods involve the use of *mollifiers*. In Selberg’s method, roughly speaking, one calculates a mollified second moment of  $\zeta(s)$  *on* the critical line, where the mollifier itself is a fourth power of an approximation to  $\zeta(s)^{1/2}$ ; see [IK04, Chapter 24.2]. In Levinson’s method, one calculates a second mollified moment of  $\zeta(s)$  *off* the critical line, where the mollifier is an approximation to  $\zeta(s)^{-1}$ .

Selberg’s method has the advantage of working regardless of the length of the mollifier. By contrast, it has long been believed that Levinson’s method suffers from a major drawback: to obtain a positive proportion of zeros on the critical line, the mollifier must be sufficiently long. This viewpoint is supported Farmer [Far94, p. 215], who provided the plot shown in Figure 1 and remarked, “It is interesting that Levinson’s method does not yield a result if  $\theta$  is too small.” Levinson’s method, however, tends to yield much stronger explicit bounds for the proportion, and in some cases, can also establish a positive proportion of simple zeros on the critical line. As described in [Iwa14, Chapter 16],

Levinson’s approach seems to be a gamble, because it is not clear up front that at the end the numerical constants are good enough to yield a positive lower bound for [the number of critical zeros up to height  $T$ ].

In this paper, we prove that Levinson’s method, as modified by Conrey [Con89], will in fact give a positive proportion of zeros on the critical line no matter how short the mollifier is—contrary to the common belief.

**1.1. Levinson’s method.** Levinson’s starting point is a theorem of Speiser [Spe35], which states that the Riemann Hypothesis is equivalent to the assertion that all non-real zeros of  $\zeta'(s)$  are in the half-plane  $\sigma \geq 1/2$ . This result was refined by Levinson and Montgomery [LM74], who proved

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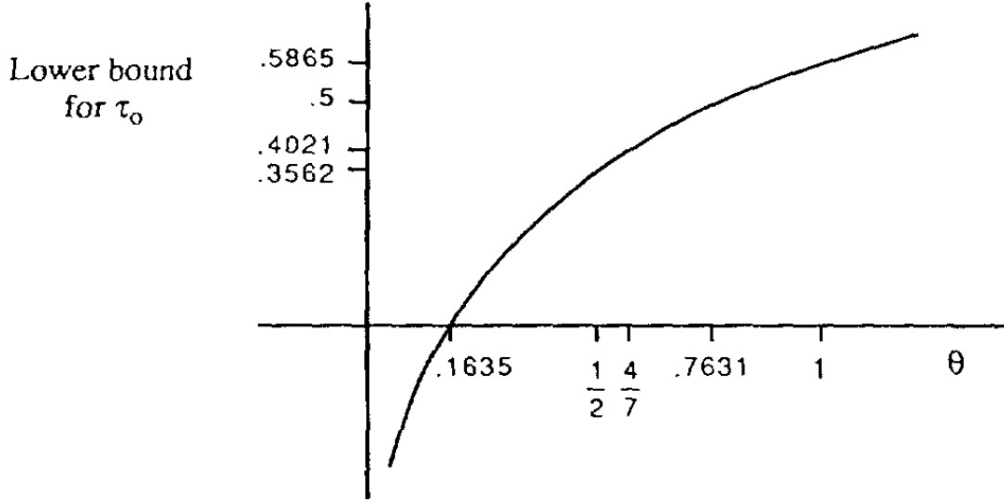


FIGURE 1. Proportion of zeros on the critical line as a function of the length  $\theta$  via Levinson's method; reprinted from [Far94, p. 215]

a (essentially) one-to-one correspondence between the non-real zeros of  $\zeta(s)$  and those of  $\zeta'(s)$  in the region  $\sigma < 1/2$  (presumably both sets are empty).

Subsequently, Levinson [Lev74] proved that the number of zeros of  $\zeta'(s)$  in the region  $\sigma < 1/2$ ,  $0 < t < T$  is at most  $(1/3)(T/2\pi) \log T$ , i.e. at most  $1/3$  of the zeros are to the *left* of  $\sigma = 1/2$ . The same result holds for  $\zeta(s)$  by the aforementioned theorem of [LM74]. The functional equation of  $\zeta(s)$  allows us to deduce that at most  $1/3$  of the zeros of  $\zeta(s)$  are to the *right* of  $\sigma = 1/2$ . This leaves *at least*  $1/3$  of the zeros of  $\zeta(s)$  *on* the line  $\sigma = 1/2$ .

Using the functional equation again, the zeros of  $\zeta'(s)$  to the left of  $\sigma = 1/2$  correspond to the zeros of  $\zeta(s) + L^{-1}\zeta'(s)$  ( $L := \log(T/2\pi)$ ) on the *right* of  $\sigma = 1/2$ . This formulation turns out to be more practical. The essential ingredient to Levinson's argument is an asymptotic formula for the moment

$$\frac{1}{T} \int_0^T |(\zeta + L^{-1}\zeta')(a + it)|^2 |M(a + it)|^2 dt, \quad (1)$$

where  $a$  is a real number slightly less than  $1/2$  (see (13)), and  $M$  is a *mollifier* of the form

$$M(s) = \sum_{n \leq y} \frac{\mu(n)}{n^{s+1/2-a}} \frac{\log(y/n)}{\log y}, \quad (2)$$

where  $\mu(n)$  is the Möbius  $\mu$ -function,  $y = T^\theta$ , and  $\theta > 0$  is the 'length' of the mollifier, the key parameter.

Levinson established (1) for all  $\theta < 1/2$ . The admissible range for  $\theta$  was later extended by Conrey [Con89] to  $\theta < 4/7$ . With refinements to be discussed below, he showed that at least 40% of the zeros of  $\zeta(s)$  are on the critical line [Con89, Theorem 1]. In [Far93], Farmer proposed the ' $\theta = \infty$ ' conjecture, that is, the admissible value for  $\theta$  can be arbitrarily large. He showed that this would imply 100% of the zeros of  $\zeta(s)$  lie on  $\sigma = 1/2$ . More recently, Bettin and Gonek [BG17] proved that ' $\theta = \infty$ ' in fact implies the Riemann Hypothesis.

Conrey [Con89] refined Levinson's method in two crucial ways. First, he observed that the role of  $\zeta(s) + L^{-1}\zeta'(s)$  in (1) can be replaced by any *linear combination* of derivatives of  $\zeta(s)$  of the

form  $Q(-\frac{1}{L} \frac{d}{ds})\zeta(s)$ , where  $Q$  is a real polynomial that satisfies

$$Q(0) = 1 \quad \text{and} \quad Q'(y) = Q'(1-y). \quad (3)$$

The condition (3) stems from the functional equation of  $\zeta(s)$ . Second, he considered a more general class of mollifiers of the form

$$M(s, P) := \sum_{n \leq y} \frac{\mu(n)}{n^{s+1/2-a}} P\left(\frac{\log(y/n)}{\log y}\right), \quad (4)$$

where  $P$  is a real polynomial with

$$P(0) = 0 \quad \text{and} \quad P(1) = 1. \quad (5)$$

He established an asymptotic formula for the corresponding mollified moment (see (12) and (15)) for any such  $P$ ,  $Q$  and  $\theta < 4/7$ , and determined the optimal choice of  $P$ .

**1.2. Results.** We prove that no matter how small  $\theta > 0$  is in (2), there exists an admissible linear combination of derivatives of  $\zeta(s)$  that yields a positive proportion of zeros of  $\zeta(s)$  on the critical line via Levinson's method. Moreover, this proportion can be made quantitative; see **Theorem 1**. In fact, our linear combination is optimal with respect to the variational problem we consider (see Problem 1 and equation (22)). Such an optimizer (for  $Q$ ) is significantly more intricate than the one for the mollifier polynomial  $P$  in [Con89, p. 9].

For small values of  $\theta$ , the improvement gained by choosing  $Q$  strategically is significant. For example, in Bernard's work [Ber15] on critical zeros of modular (degree two)  $L$ -functions, he obtains a proportion of 2.97% of zeros on  $\sigma = 1/2$  (using the optimal  $P$  and an empirical  $Q$  of degree 7), whereas we get 6.32% (using  $P(x) = x$  and our newly constructed  $Q$ ), both unconditionally and using the same shifted convolution estimate. We have not attempted to optimize the proportion here (a method for full optimization is described in Section 7), but our result already comes close to the current record achieved in [AT21] (using the optimal  $P$  and an empirical  $Q$  of degree 27!).

The broader goal is to initiate a systematic and *theoretical* study of how to select effective linear combinations of derivatives of the  $\zeta$ - (or  $L$ -) functions in analytic applications, in contrast to the predominantly *empirical*, computer-experimental approach used to date.

**1.3. Connections to Siegel's method.** Let  $h(s) := \pi^{-s/2} \Gamma(s/2)$ . Levinson's method detects zeros of  $\zeta(s)$  on  $\sigma = 1/2$  by identifying when  $\arg(h\zeta')(1/2 + it) \equiv \pi/2 \pmod{\pi}$  occurs. By the argument principle, this task reduces to bounding the number of zeros of  $\zeta'(s)$  on  $\sigma < 1/2$ . In the introduction to [Lev74], Levinson noted that the idea of detecting zeros of  $\zeta(s)$  on the critical line via changes in argument and moment estimates (of a suitable function) had been used in Siegel's 1932 work [Sie32].

In [Sie32], instead of working with  $\zeta'(s)$  as in [Lev74], Siegel introduced an interesting entire function:

$$\mathfrak{f}(s) := \int_L \frac{e^{i\pi w^2}}{e^{i\pi w} - e^{-i\pi w}} w^{-s} dw, \quad (6)$$

where the line of integration  $L$  has slope 1, with  $\text{Im } w$  decreasing, and intersects the real axis at a point between 0 and 1. The function  $\mathfrak{f}(s)$  originates from the *Riemann–Siegel formula*, which is an integral representation of  $\zeta(s)$  given by

$$h(s)\zeta(s) = 2 \operatorname{Re} h(s)\mathfrak{f}(s) \quad (\operatorname{Re} s = 1/2). \quad (7)$$

This formula first appeared in Riemann's 1859 memoir [Rie] but remained largely unnoticed in the literature until its rediscovery by Siegel.

Whenever  $\arg(hf)(1/2+it) \equiv \pi/2 \pmod{\pi}$  occurs, it follows from (7) that there is a zero of  $\zeta(s)$  on the critical line. In fact, Siegel proved that

$$N_0(T) > 2 \cdot \#\{s = \sigma + it : f(s) = 0, \sigma < 1/2, 0 < t < T\}, \quad (8)$$

where  $N_0(T)$  is the number of zeros of  $\zeta(s)$  with  $\sigma = 1/2$  with  $0 < t \leq T$ . A *lower bound* to the right-hand side of (8) can be obtained by evaluating the moment

$$\frac{1}{T} \int_1^T |f(\sigma + it)|^2 dt, \quad (9)$$

which turns out to be  $\sim C_\sigma \cdot T^{1/2-\sigma}$  for some explicit  $C_\sigma > 0$ , and for  $\sigma < 1/2$  to be chosen. As a consequence, Siegel established, for  $T \gg 1$ , that

$$N_0(T) > \frac{3}{8\pi} e^{-3/2} T, \quad (10)$$

which improves upon the result of Hardy and Littlewood [HL21] that  $N_0(T) \gg T$ .

The function  $f(s)$  can be *formally* interpreted in Conrey–Levinson’s set-up. Consider

$$Q_\infty(y) := \begin{cases} 1 & \text{if } 0 \leq y < 1/2 \\ 1/2 & \text{if } y = 1/2 \\ 0 & \text{if } 1/2 < y \leq 1. \end{cases} \quad (11)$$

Let  $s = 1/2 + iT$  with  $T \gg 1$ , and  $L := \log(T/2\pi)$ . By the saddle point method, Siegel deduced, up to a negligible error of  $O(T^{-1/4})$ , that

$$f(s) = \sum_{n \leq \sqrt{T/2\pi}} \frac{1}{n^s} = \sum_{n=1}^{\infty} n^{-s} Q_\infty\left(\frac{\log n}{L}\right) = \sum_{n=1}^{\infty} Q_\infty\left(-\frac{1}{L} \frac{d}{ds}\right) n^{-s} = Q_\infty\left(-\frac{1}{L} \frac{d}{ds}\right) \zeta(s).$$

The step function  $Q_\infty(y)$  satisfies the condition (3) apart from failing to be differentiable at  $y = 1/2$ , and therefore does not qualify as an admissible function in Conrey–Levinson’s method. In fact, it was commented in [Lev74, p. 384] that

It appears to me that the function  $f_1(s)$  [i.e.,  $f(s)$ ] is not amenable to improvement with a mollifier.

As Siegel noted at the end of his paper, his method itself *cannot* yield a bound  $N_0(T) \gg T(\log \log T)^{1+\epsilon}$ . However, we will show that

**Proposition 1.** *For any  $\theta > 0$ , let  $Q_\theta : [0, 1] \rightarrow \mathbb{R}$  be the function constructed in Theorem 1, which is used to define linear combinations of derivatives of  $\zeta(s)$ . Then as  $\theta \rightarrow 0+$ , the pointwise limit of  $Q_\theta(y)$  converges to the step function  $Q_\infty(y)$  for any  $y \in [0, 1]$ .*

In other words, behind **Theorem 1** is the idea of mollifying linear combinations of derivatives of  $\zeta(s)$  that *approximate* Siegel’s function  $f(s)$ . Proposition 1 shows that we are actually using polynomials  $Q$  of *arbitrarily large* degree in showing Levinson’s method works for mollifiers of any length  $\theta > 0$ . Unlike previous works on mollifiers and critical zeros, a key feature of our approach is that our linear combinations vary with the values of  $\theta$ .

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All computations and plots in this article were carried out using *Mathematica*. The relevant commands are included in Appendix A. The corresponding dataset (.mx files) and notebooks (.nb files) are available at <https://github.com/davidfarmer/shortmollifiers>.

## 2. PRELIMINARY WORK

**2.1. Set up.** Let  $P$  be a polynomial satisfying (5),  $Q$  a polynomial satisfying (3), and let  $R > 0$  be any constant. According to [Con89, eq. (39)], if  $\theta > 0$  is an admissible constant such that the asymptotic formula

$$\frac{1}{T} \int_0^T \left| Q\left(-\frac{1}{L} \frac{d}{ds}\right) \zeta(a+it) M(a+it, P) \right|^2 dt \sim c(P, Q, R) \quad (12)$$

holds as  $T \rightarrow \infty$ , where

$$a = 1/2 - R/\log(T/2\pi), \quad (13)$$

and  $c(P, Q, R)$  is a constant depending on  $P, Q$ , and  $R$ , then the proportion of zeros of  $\zeta(s)$  on the critical line is *at least*

$$\kappa := 1 - \frac{\log c(P, Q, R)}{R}. \quad (14)$$

By [Con89, Theorem 2], the constant  $c(P, Q, R)$  is given by

$$1 + \frac{1}{\theta} \int_0^1 \int_0^1 (w(y)P'(x) + \theta w'(y)P(x))^2 dx dy, \quad (15)$$

where

$$w(y) := e^{Ry} Q(y). \quad (16)$$

To simplify the exposition and illustrate the strength of our construction, we adopt Levinson's original choice:

$$P(x) = x. \quad (17)$$

Also, observe that the class of admissible functions  $Q$  can be extended to include all continuously differentiable ( $C^1$ ) functions  $Q : [0, 1] \rightarrow \mathbb{R}$  with

$$Q(0) = 1 \quad \text{and} \quad Q(y) + Q(1-y) = 1. \quad (18)$$

Indeed, it follows from the Weierstrass approximation theorem that any such  $Q$  can be uniformly approximated by sequences of polynomials on  $[0, 1]$  that satisfy (18).

We now state our main result.

**Theorem 1.** *There exists  $\theta_0 > 0$  such that whenever  $\theta \in (0, \theta_0)$ , there exists  $Q = Q_\theta \in C^1[0, 1]$  satisfying (18) such that  $\kappa$  defined in (14) satisfies  $\kappa > 2\theta/3 > 0$ .*

The constant  $\theta_0$  is explicitly computable. In fact, our numerical evidence (see Figure 7b) suggests the following explicit bound for any  $0 < \theta \leq 1/2$ :

$$\kappa > (2/3)\theta. \quad (19)$$

Moreover, we will be able to make more general choices of  $P$  and  $Q$  in Section 7.

**2.2. Simplification.** Expanding the square of (15) and integrating the mixed term with the identity  $\int_0^1 f(x)f'(x) dx = (f(1)^2 - f(0)^2)/2$ , we have

$$c(P, Q, R) = \frac{1}{2} + J(Q), \quad (20)$$

where  $J(Q)$  is the functional

$$J(Q) = J_{R,\theta}(Q) := \int_0^1 \left( \frac{1}{\theta} w(y)^2 + \frac{\theta}{3} w'(y)^2 \right) dy, \quad (21)$$

and  $w(y)$  is defined in (16). Given constants  $R, \theta > 0$ , we aim to find the minimum of  $J(Q)$  subject to the condition (18).

The expressions can be simplified by some changes of variables. Letting

$$q(y) := Q(y + 1/2) \quad \text{and} \quad S(t) = S_R(t) := q(t/2R) \quad (22)$$

in (21), we have

$$J(Q) = \frac{e^R}{2R} \int_{-R}^R \left( \frac{1}{\theta} e^t S(t)^2 + \frac{\theta}{3} R^2 e^t (S(t) + 2S'(t))^2 \right) dt, \quad (23)$$

and the condition (18) becomes

$$S(-R) = 1 \quad \text{and} \quad S(t) + S(-t) = 1. \quad (24)$$

Here,  $S$  is a real-valued,  $C^1$ -function defined on  $[-R, R]$ . It follows that  $S(R) = 0$ , and, in particular, that

$$\int_{-R}^R e^t S(t) S'(t) dt = -\frac{e^{-R}}{2} - \frac{1}{2} \int_{-R}^R e^t S(t)^2 dt.$$

Hence, we may write

$$J(Q) = -\frac{\theta}{3} R + \frac{e^R}{2R} K(S), \quad (25)$$

where

$$K(S) = K_{\theta,R}(S) := \int_{-R}^R e^t [c_0 S(t)^2 + c_1 S'(t)^2] dt, \quad (26)$$

and the constants  $c_0, c_1$  are given by

$$c_0 = c_0(R, \theta) := \frac{1}{\theta} - \frac{\theta}{3} R^2 \quad \text{and} \quad c_1 = c_1(R, \theta) := \frac{4\theta}{3} R^2. \quad (27)$$

By splitting the integral in (26) into the part from  $-R$  to  $0$  and the part from  $0$  to  $R$ , we may impose the constraint  $S(t) + S(-t) = 1$  and further simplify  $K(S)$  to write

$$K(S) = \int_0^R \left( e^t (c_0 S(t)^2 + c_1 S'(t)^2) + e^{-t} (c_0 (1 - S(t))^2 + c_1 S'(t)^2) \right) dt. \quad (28)$$

We have reduced the problem to finding the minimizer of  $K(S)$  subject to (24).

To keep our argument clean and reduce the number of variables in the course of proving Theorem 1, we introduce the following assumption:

**Assumption 1.** Assume that  $c_0 = c_1$ , where  $c_0, c_1$  are defined in (27).

We emphasize, however, that the steps leading up to Section 3.1 do not depend on this assumption. A generalization is given in Section 7. The computations following Section 3.1 can also be extended to the general case, though at the expense of increased computational complexity.

The assumption is equivalent to

$$\theta = R^{-1} \sqrt{\frac{3}{5}}. \quad (29)$$

In this case, we have  $c_0 = c_1 = 4/(5\theta)$ . We note that  $R$  can be taken to be any positive constant. We insert (29) into (28) to write

$$K_R^*(S) := \frac{4}{5\theta} \int_0^R e^t (S(t)^2 + S'(t)^2) + e^{-t} ((1 - S(t))^2 + S'(t)^2) dt. \quad (30)$$

Here, ‘ $*$ ’ in  $K_R^*(S)$  signifies the use of (29). Our main problem can now be stated as follows.

**Problem 1.** *Given any  $R > 0$ , find the minimum value of the functional  $K_R^*(S)$  and the minimizer  $S = S_R(t)$  subject to the condition (24).*

In the next section, we solve this problem by using the calculus of variations.

### 3. CALCULUS OF VARIATIONS

In the following, we write  $K^*(S) = K_R^*(S)$ . Suppose that  $K^*(S)$  attains a minimum at  $S$ , and let  $\epsilon > 0$  be small and  $\phi(t)$  be an arbitrary smooth test function on  $[0, R]$  such that  $\phi(0) = \phi(R) = 0$ . Then  $K^*(S + \epsilon\phi)$ , as a function of  $\epsilon$ , has a minimum at  $\epsilon = 0$ . Since

$$\begin{aligned} \left. \frac{d}{d\epsilon} K^*(S + \epsilon\phi) \right|_{\epsilon=0} &= \frac{4}{5\theta} \int_0^R (e^t (2S\phi + 2S'\phi') + e^{-t} (2(S-1)\phi + 2S'\phi')) dt \\ &= \frac{16}{5\theta} \int_0^R (\cosh(t)S(t) - (S'(t)\cosh t)' - \frac{1}{2}e^{-t})\phi(t) dt, \end{aligned}$$

we must determine  $S$  for which the Euler–Lagrange equation

$$\frac{d}{dt} (S' \cosh t) = S \cosh t - \frac{1}{2}e^{-t} \quad (31)$$

is satisfied. Equation (31) can be rewritten as

$$S''(t) + (\tanh t)S'(t) - (S(t) - \frac{1}{1+e^{2t}}) = 0. \quad (32)$$

The boundary conditions for (32) are

$$S(0) = 1/2 \quad \text{and} \quad S(R) = 0. \quad (33)$$

Before proceeding to solve for  $S$ , we incorporate the preceding steps to rewrite  $c(P, Q, R)$  as defined in (20). Assume that  $S$  satisfies the differential equation (31). Then

$$\begin{aligned} \int_0^R S'(t)^2 \cosh t dt &= S(t)S'(t)\cosh t \Big|_0^R - \int_0^R S(t) \frac{d}{dt} (S'(t)\cosh t) dt \\ &= -\frac{1}{2}S'(0) - \int_0^R S(t) (S(t)\cosh t - \frac{1}{2}e^{-t}) dt. \end{aligned}$$

It follows from (28) that

$$\begin{aligned} K^*(S) &= \frac{8}{5\theta} \int_0^R (S(t)^2 \cosh t + S'(t)^2 \cosh t - e^{-t} S(t)) dt + \frac{4}{5\theta} (1 - e^{-R}) \\ &= \frac{4}{5\theta} \left( 1 - e^{-R} - S'(0) - \int_0^R e^{-t} S(t) dt \right). \end{aligned} \quad (34)$$

Upon substituting (29) and (34) into (25), we find that (20) becomes

$$\begin{aligned} c(P, Q, R) &= \frac{1}{2} - \frac{\theta}{3} R + \frac{e^R}{2R} \frac{4}{5\theta} \left( 1 - e^{-R} - S'(0) - \int_0^R e^{-t} S(t) dt \right) \\ &= \frac{1}{2} + \frac{1}{\sqrt{15}} \left( -1 + 2e^R (1 - e^{-R} - S'(0) - \int_0^R e^{-t} S(t) dt) \right). \end{aligned} \quad (35)$$

Readers should keep in mind that (35) depends only on  $R$  because of (29) and (17).

**3.1. Solving the Euler–Lagrange equation.** We first present the solution to the differential equation

$$\begin{cases} S''(t) + \tanh(t)S'(t) - S(t) + (1 + e^{2t})^{-1} = 0, \\ S(0) = 1/2, \quad \text{and} \quad S(R) = 0. \end{cases} \quad (36)$$

It takes the form

$$S_R(t) := C_1(R)f(t) + g_0(t) + g_1(t) \int_0^t v_1(u) du + g_2(t) \int_0^t v_2(u) du, \quad (37)$$

where the functions  $C_1, f, g_0, g_1, g_2, v_1$  and  $v_2$  are all expressible in terms of the Gauss  ${}_2F_1$ -hypergeometric function

$${}_2F_1(a, b, c; z) := \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!}. \quad (38)$$

The series (38) converges for  $|z| < 1$  and  $a, b, c \in \mathbb{C}$  with  $c \neq 0, -1, -2, \dots$ , and it admits an analytic continuation in the  $z$ -variable over  $\mathbb{C} - [1, +\infty)$ . We also record Euler's reflection formula, which states

$$\Gamma(s)\Gamma(1-s) = \frac{\pi}{\sin(\pi s)}, \quad s \notin \mathbb{Z}. \quad (39)$$

The component functions of  $S_R(t)$  are defined as follows. To simplify the typesetting, we define  $\phi := (1 + \sqrt{5})/2$ ;

$$\begin{aligned} F^+(t) &:= {}_2F_1(1/2, \phi, 1/2 + \phi, -e^{2t}); \quad F^-(t) := {}_2F_1(1/2, -\phi^{-1}, 1/2 - \phi^{-1}, -e^{2t}), \\ F_1^+(u) &:= {}_2F_1(1/2, 1 + \phi, 1/2 + \phi, -e^{2u}), \quad F_1^-(u) := {}_2F_1(3/2, -\phi^{-1}, 1/2 - \phi^{-1}, -e^{2u}). \end{aligned}$$

The various components appearing on the right-hand side of (37) are given by:

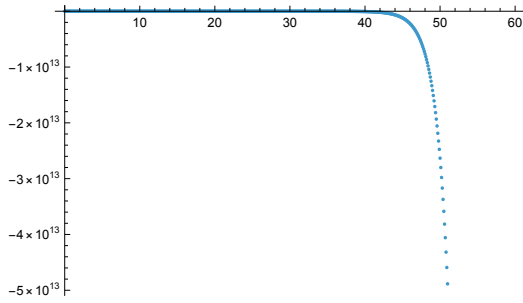
$$g_1(t) = e^{-\phi^{-1}t} F^-(t), \quad g_2(t) = e^{\phi t} F^+(t), \quad f(t) = g_1(t) - \frac{g_1(0)}{g_2(0)} g_2(t), \quad g_0(t) = \frac{1}{2} \frac{g_2(t)}{g_2(0)},$$

$$v_1(u) = \frac{g_2(u)}{\mathcal{W}(u)(1 + e^{2u})}, \quad v_2(u) = -\frac{g_1(u)}{\mathcal{W}(u)(1 + e^{2u})},$$

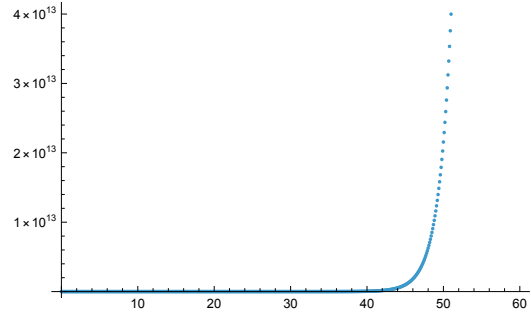
and

$$C_1(R) = \frac{-2F^-(R)F^+(0)w_1(R) - e^{\sqrt{5}R}F^+(R)(1 + 2F^+(0)w_2(R))}{2F^-(R)F^+(0) - 2e^{\sqrt{5}R}F^-(0)F^+(R)}, \quad (40)$$

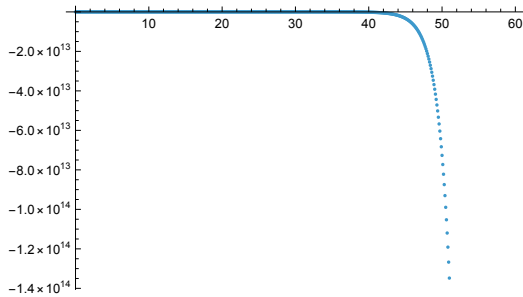




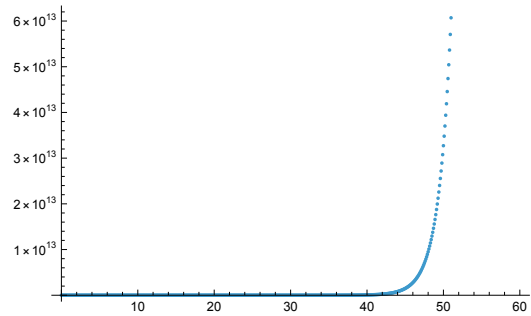
Plot for  $f(t)$



Plot for  $g_0(t)$



Plot for  $g_1(t)$



Plot for  $g_2(t)$

where  $w_1(t) := \int_0^t v_1(u) du$ ,  $w_2(t) := \int_0^t v_2(u) du$ , and

$$\mathcal{W}(u) := e^u (2\phi F^-(u) F_1^+(u) - F^+(u) F_1^-(u)). \quad (41)$$

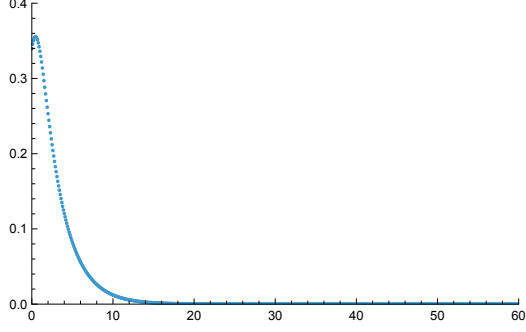
Thus,  $S_R(t)$  is fully described, and plots of its component functions are included.

We now derive (37). Recall that the  ${}_2F_1$ -hypergeometric function can be characterized by a second-order linear homogeneous differential equation [DLMF, eq. (15.10.1)]. By a simple change of variables, one may readily observe (or check) that a set of fundamental solutions to the homogeneous differential equation  $S''(t) + \tanh(t)S'(t) - S(t) = 0$  is given by  $\{g_1(t), g_2(t)\}$ . Its Wronskian can be computed to be exactly  $\mathcal{W}(u)$  defined in (41).

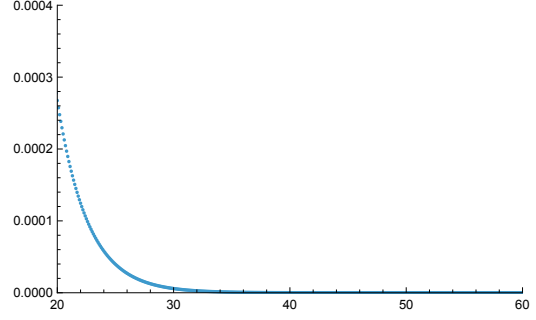
The standard method of *variation of parameters* (see [CL55, Chapter 3]) may now be used to solve our desired inhomogeneous equation (36), which asserts that the sum of the last two terms on the right side of (37) satisfies such a differential equation. The first two terms on the right side, which clearly satisfy the homogeneous equation, are included to ensure the boundary conditions are satisfied. Indeed,  $f(0) = 0$  and  $g_0(0) = 1/2$ , and  $C_1(R)$  is defined such that  $S(R) = 0$ . Altogether, these yield a solution of the form (37). Indeed, a direct *Mathematica* check (`ODE_Check.nb`) confirms that (37) satisfies (36).

**3.2. Evaluating the components of  $S_R(t)$ .** We now record the leading order asymptotics of the above quantities (as  $t, u, R \rightarrow \infty$ ), computed with *Mathematica* (see the notebook `Asymp.nb`<sup>1</sup>). These asymptotics will be used in Section 5 to complete the proof of Theorem 1. We first apply

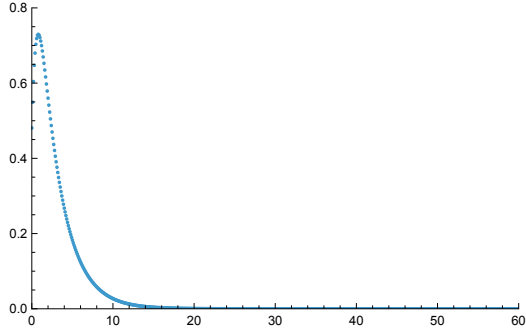
<sup>1</sup>The commands used in the notebooks are also documented in Appendix A.



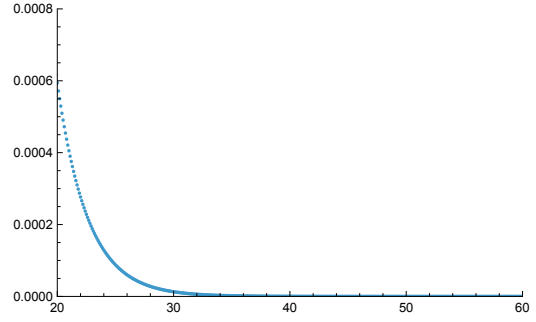
Plot for  $v_1(u)$  from 0 to 60



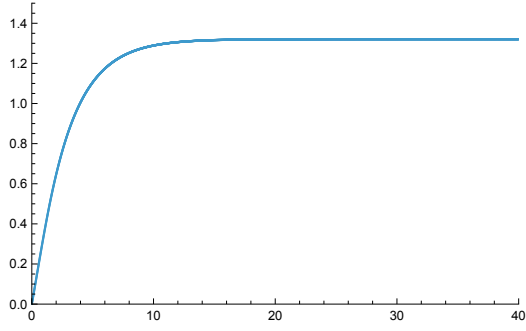
Plot for  $v_1(u)$  from 20 to 60



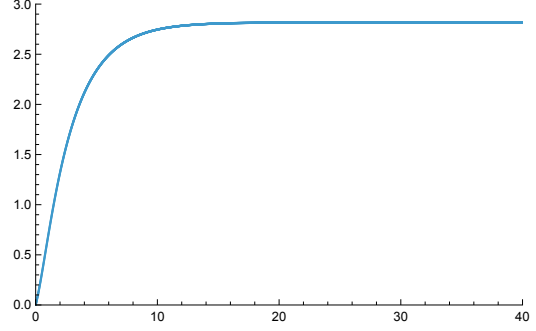
Plot for  $v_2(u)$  from 0 to 60



Plot for  $v_2(u)$  from 20 to 60



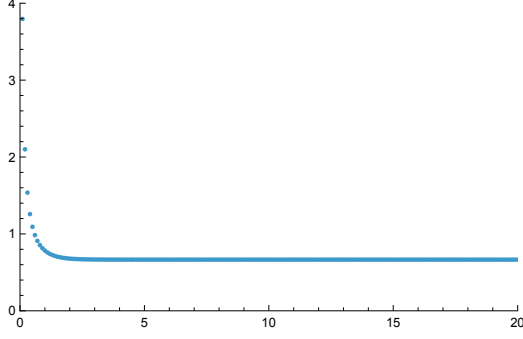
Plot for  $w_1(t)$  from 0 to 40



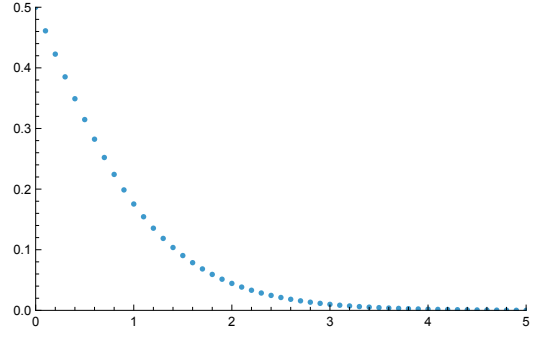
Plot for  $w_2(t)$  from 0 to 40

[DLMF, eq. (15.8.2)], which for real  $z < 0$  states

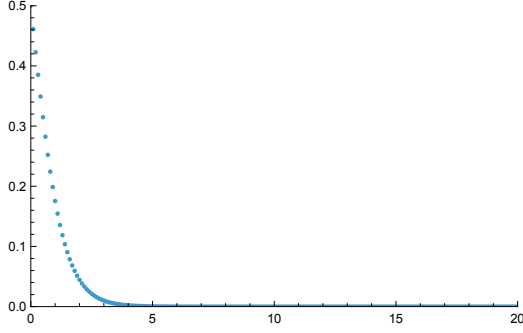
$$\begin{aligned}
& \frac{\sin \pi(b-a)}{\pi \Gamma(c)} {}_2F_1(a, b, c; z) \\
&= \frac{(-z)^{-a}}{\Gamma(b)\Gamma(c-a)\Gamma(a-b+1)} {}_2F_1\left(a, a-c+1, a-b+1; \frac{1}{z}\right) \\
&\quad - \frac{(-z)^{-b}}{\Gamma(a)\Gamma(c-b)\Gamma(b-a+1)} {}_2F_1\left(b, b-c+1, b-a+1; \frac{1}{z}\right). \tag{42}
\end{aligned}$$



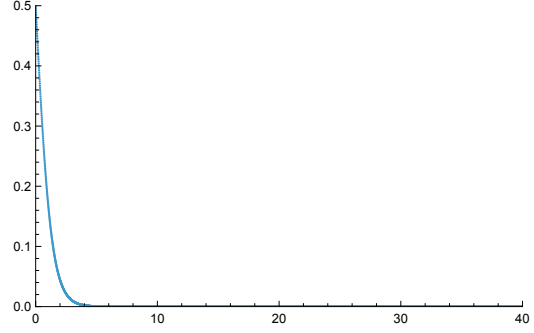
Plot for  $C_1(R)$



Plot for  $S_R(t)$  with  $R = 5$



Plot for  $S_R(t)$  with  $R = 20$



Plot for  $\lim_{R \rightarrow \infty} S_R(t)$

In our setting,  $z = -e^{2t}$ , where  $t \geq 0$ , and  $a, b$ , and  $c$  are non-integer real numbers. Thus by (42), the power series (38), and the reflection formula (39), we have the full expansion

$$\begin{aligned} & \frac{\sin \pi(b-a)}{\Gamma(c)} {}_2F_1(a, b, c; -e^{2t}) \\ &= \frac{e^{-2ta} \sin \pi(c-a)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(a-c+1+n)}{\Gamma(a-b+1+n)} \frac{(-e^{-2t})^n}{n!} \\ & \quad - \frac{e^{-2tb} \sin \pi(c-b)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(b+n)\Gamma(b-c+1+n)}{\Gamma(b-a+1+n)} \frac{(-e^{-2t})^n}{n!}. \end{aligned} \quad (43)$$

Note that (43) implies, as  $t \rightarrow \infty$ , that  ${}_2F_1(a, b, c; -e^{2t}) = O(e^{-2t \min\{a, b\}})$ . Using (43), we may use *Mathematica* to determine the leading-order asymptotics for the functions making up  $S_R(t)$  efficiently and precisely. First, as  $t \rightarrow \infty$ , we have <sup>2</sup>

$$F^+(t) \sim 1.2427 \dots e^{-t} \quad \text{and} \quad F^-(t) \sim -2.75957 \dots e^{(\sqrt{5}-1)t}$$

so that

$$g_1(t) \sim -2.75957 \dots e^{\frac{\sqrt{5}-1}{2}t}, \quad g_2(t) \sim 1.2427 \dots e^{\frac{\sqrt{5}-1}{2}t},$$

$$f(t) \sim -e^{\frac{\sqrt{5}-1}{2}t} \quad \text{and} \quad g_0(t) \sim 0.81855 \dots e^{\frac{\sqrt{5}-1}{2}t}.$$

Next, as  $u \rightarrow \infty$ , we have

$$F_1^+(u) \sim 0.85875 \dots e^{-u} \quad \text{and} \quad F_1^-(u) \sim -6.17059 \dots e^{(\sqrt{5}-1)u}$$

<sup>2</sup>In this article, the decimal values given are truncations of the actual values.

so that

$$v_1(u) \sim 0.55579 \dots e^{-\frac{3-\sqrt{5}}{2}u} \quad \text{and} \quad v_2(u) \sim 1.23411 \dots e^{-\frac{3-\sqrt{5}}{2}u}.$$

It is now clear that  $\lim_{R \rightarrow \infty} w_i(R)$  exist for  $i = 1, 2$ .

**Remark 1.** *The coefficients appearing in the asymptotics above can indeed be expressed in closed form. For example, we have  $1.2427 \dots = \Gamma(1 + \sqrt{5}/2)\Gamma(\sqrt{5}/2)/\Gamma((1 + \sqrt{5})/2)^2$  and  $-2.75957 \dots = \csc(\sqrt{5}\pi/2)$ , which follow readily from the Pfaff transformation formula [DLMF, eq. (15.8.1)], the Gauss summation formula [DLMF, eq. (15.4.20)], and the Euler reflection formula (39).*

Finally, we have that the numerator and denominator of  $C_1(R)$  are both  $\asymp e^{(\sqrt{5}-1)R}$ , and thus the limit of  $C_1(R)$  as  $R \rightarrow \infty$  exists. Indeed, by *Mathematica*, we find that

$$w_1(\infty) = 1.3208 \dots \quad \text{and} \quad w_2(\infty) = 2.8166 \dots \quad (44)$$

Thus,

$$C_1(R) \sim \frac{4.18979 \dots w_1(\infty) - 1.2428 \dots - 1.88691 \dots w_2(\infty)}{-1.51827 \dots} \sim 0.674 \dots \quad (45)$$

Once again, the constants  $4.18979 \dots$ ,  $1.2428 \dots$ ,  $1.88691 \dots$ , and  $1.51827 \dots$  appearing in (45) can be expressed in terms of the  $\Gamma$ -functions and the  ${}_2F_1$ -hypergeometric functions evaluated at  $z = -1$ . Also, we note that the function  $\lim_{R \rightarrow \infty} S_R(t)$  is of the order  $e^{\frac{\sqrt{5}-1}{2}t}$ .

**Remark 2.** *For the readers' convenience, we have generated tables of values for:*

- $v_1(u)$ ,  $v_2(u)$  over the interval  $u \in [0, 40]$  with step size = 1/5000  
(files: `Tbv140oneOver5000.mx`, `Tbv240oneOver5000.mx`);
- $w_1(t)$ ,  $w_2(t)$  over the interval  $t \in [0, 40]$  with step size = 1/100  
(files: `Tbw140ref1over100.mx`, `Tbw240ref1over100.mx`);
- $C_1(R)$  over the interval  $R \in [0, 40]$  with step size = 1/100  
(file: `ConstC40oneOver100.mx`);
- $\lim_{R \rightarrow \infty} S_R(t)$  over the interval  $t \in [0, 40]$  with step size = 1/100  
(file: `Sinf40oneOver100.mx`).

*These datasets can be generated by the notebook `Pre_compute.nb`. The graphs included can be created with the standard plotting functions `Plot[]` and `ListPlot[]` (or see `Plot.nb`).*

#### 4. RELATION TO SIEGEL'S FUNCTION: PROOF OF PROPOSITION 1

Recall from (22) that  $Q_R(y) = S_R(2R(y - 1/2))$ . The initial condition in (36) implies that  $Q_R(1/2) = 0$ . By (24), it suffices to consider the range  $1/2 < y \leq 1$ .

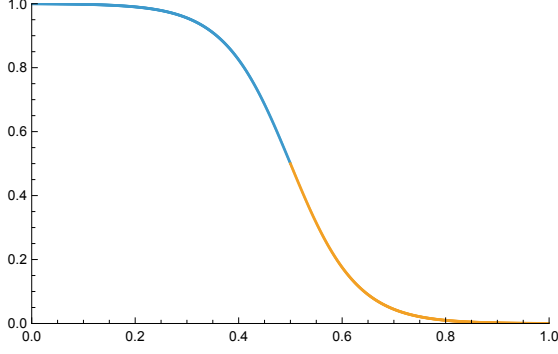
Let  $y_0 \in (1/2, 1]$  be given. We have determined that  $f(t)$ ,  $g_0(t)$ ,  $g_1(t)$ ,  $g_2(t)$  all exhibit the same asymptotic order  $e^{\frac{\sqrt{5}-1}{2}t}$  as  $t \rightarrow \infty$ . Then for any  $\mathcal{F} \in \{f, g_0, g_1, g_2\}$ , we have

$$\lim_{R \rightarrow \infty} \mathcal{F}(t) e^{-\frac{\sqrt{5}-1}{2}t} \Big|_{t=2R(y_0-1/2)} = \lim_{R \rightarrow \infty} \mathcal{F}(t) e^{-\frac{\sqrt{5}-1}{2}t} \Big|_{t=R}. \quad (46)$$

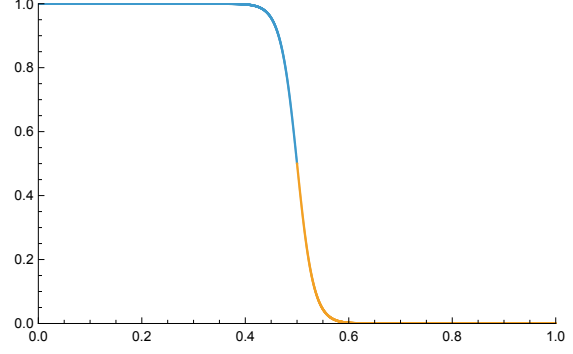
Also, it is clear that  $\lim_{R \rightarrow \infty} w_i(2R(y_0 - 1/2)) = \lim_{R \rightarrow \infty} w_i(R) = w_i(\infty)$  for  $i = 1, 2$ . Now, using (37), (45) and the initial condition, we conclude that

$$\lim_{R \rightarrow \infty} S_R(t) e^{-\frac{\sqrt{5}-1}{2}t} \Big|_{t=2R(y_0-1/2)} = \lim_{R \rightarrow \infty} S_R(R) e^{-\frac{\sqrt{5}-1}{2}R} = 0, \quad (47)$$

and thus,  $\lim_{R \rightarrow \infty} Q_R(y_0) = 0$ . This completes the proof.



(A) Plot for  $Q_5(y)$



(B) Plot for  $Q_{20}(y)$

## 5. PROOF OF THEOREM 1

Our goal is to show that

$$\kappa = \kappa(\theta) := 1 - \frac{\log c(P, Q, R)}{R} > 0, \quad (48)$$

where  $\theta = R^{-1}\sqrt{3/5}$ ,  $P(x) = x$ ,  $Q(y) = Q_R(y) = S_R(2R(y - 1/2))$ , and

$$c(P, Q, R) = \frac{1}{2} - \frac{1}{\sqrt{15}} + \frac{2}{\sqrt{15}} e^R \left( 1 - e^{-R} - S'_R(0) - \int_0^R e^{-t} S_R(t) dt \right), \quad (49)$$

which depends only on  $R$  (or equivalently,  $\theta$ ). In particular, we seek an upper bound for the expression enclosed in  $(\dots)$  in (49).

The asymptotics given in Section 3.2 imply that the following integrals converge absolutely. Moreover, their numerical values can be computed with `Integral.kappa.nb`:

$$\begin{aligned} \int_0^\infty e^{-t} f(t) dt &= -2.1166\dots, & \int_0^\infty e^{-t} g_0(t) dt &= 1.9453\dots, \\ \int_0^\infty e^{-t} g_1(t) \int_0^t v_1(u) du dt &= -4.294\dots, & \int_0^\infty e^{-t} g_2(t) \int_0^t v_2(u) du dt &= 4.024\dots \end{aligned}$$

From these and (37), it follows that

$$\int_0^R e^{-t} S_R(t) dt = -2.1166\dots C_1(R) + 1.675\dots, \quad (50)$$

and

$$\lim_{R \rightarrow \infty} \int_0^R e^{-t} S_R(t) dt \geq 0.248. \quad (51)$$

Also, we have the numerical values

$$\begin{aligned} f'(0) &= -1.47277\dots, & g'_0(0) &= 0.602775\dots, & g_1(0) &= -1.07479\dots, \\ g_2(0) &= 0.759136\dots, & v_1(0) &= 0.339496\dots, & v_2(0) &= 0.480664\dots \end{aligned} \quad (52)$$

By (37), (45) and the evaluation above, we obtain

$$\begin{aligned} S'_R(0) &= C_1(R) f'(0) + g'_0(0) + g_1(0) v_1(0) + g_2(0) v_2(0) \\ &= -1.47277\dots C_1(R) + 0.60277\dots \end{aligned} \quad (53)$$

and

$$\lim_{R \rightarrow \infty} S'_R(0) \geq -0.39006. \quad (54)$$

Therefore, from (50) and (53), we have

$$1 - e^{-R} - S'_R(0) - \int_0^R e^{-t} S_R(t) dt = -e^{-R} + 3.58938 \dots C_1(R) - 1.278 \dots \quad (55)$$

By (51) and (54), we have

$$\lim_{R \rightarrow \infty} (1 - e^{-R} - S'_R(0) - \int_0^R e^{-t} S_R(t) dt) \leq 1.1421.$$

Since  $R = \theta^{-1} \sqrt{3/5}$ , there exists  $\theta_0 > 0$  such that for all  $0 < \theta < \theta_0$ , we have

$$1 - e^{-R} - S'_R(0) - \int_0^R e^{-t} S_R(t) dt \leq 1.2,$$

and

$$c(P, Q, R) \leq \frac{1}{2} + \frac{1}{\sqrt{15}}(2.2842e^R - 1) \leq 0.5898e^R + 0.242 \leq 0.5898e^R(1 + 0.411e^{-R}).$$

Using the elementary inequality  $\log(1 + x) \leq x$  for  $x > -1$ , it follows that

$$\kappa \geq \frac{1}{R}(-\log 0.5898 - 0.411e^{-R}). \quad (56)$$

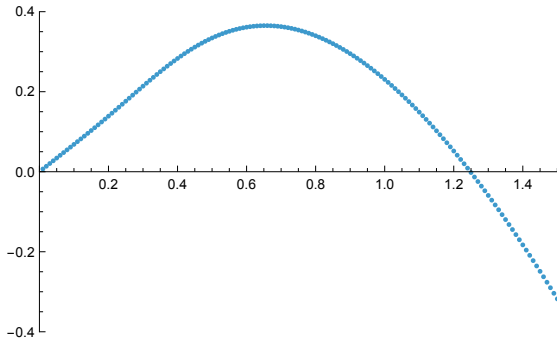
There exists  $\theta_1 > 0$  such that whenever  $0 < \theta < \theta_1$  we have  $0.411e^{-R} < 0.0001$ . Thus,

$$\kappa \geq \theta \sqrt{\frac{5}{3}}(-\log 0.5898 - 0.0001) \geq 2\theta/3. \quad (57)$$

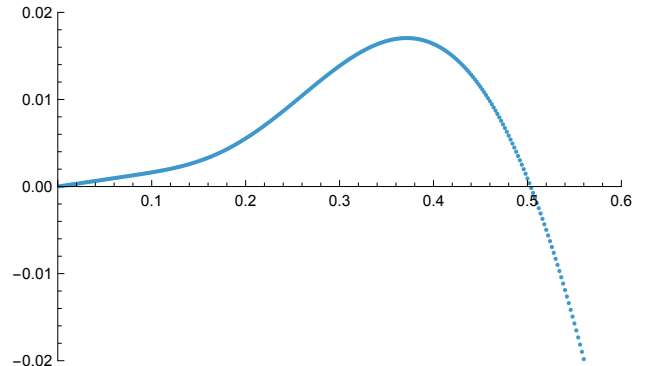
for  $0 < \theta < \min\{\theta_0, \theta_1\}$ . In particular, there is a positive proportion of zeros for  $\zeta(s)$  for sufficiently small  $\theta > 0$ . This completes the proof of Theorem 1.

## 6. SOME DATA

We record the proportions  $\kappa = \kappa(\theta)$  of zeros of  $\zeta(s)$  on  $\text{Re } s = 1/2$  using (14), (35), and (37) for various values of  $\theta$ . Here are the plots and numerics (generated with `Integral.kappa.nb`):



(A) Plot for  $\kappa(\theta)$  with  $P(x) = x$ ,  $Q(x) = Q_R(x)$ ,  $R = \theta^{-1} \sqrt{3/5}$



(B) Plot for  $\kappa(\theta) - (2/3)\theta$

$\theta$	$\kappa$
2/3	0.364...
1/2	0.334...
1/4	0.176...
1/6	0.114...
1/8	0.0854...
5/54 = 0.092...	0.0632...
1/100	0.00682...
1/500	0.00136...

The values 5/54 and 1/8 in our table for the  $\zeta$ -function are of interest as they correspond to 5/27 and 1/4 for modular  $L$ -functions in [Ber15] and [KRZ19], based on the well-known principle that a mollifier of length  $\theta$  for a  $\mathrm{GL}(n)$   $L$ -function corresponds to a mollifier of length  $\theta/n$  for a  $\mathrm{GL}(1)$   $L$ -function; see [Far94, pp. 215-216] and [Ber15, Theorem 5]. The proportions of 0.0297 and 0.0297607 were obtained unconditionally in [Ber15] and [KRZ19], respectively, and 0.0693 and 0.0693872 assuming the Ramanujan–Selberg conjecture (RSC). (It is worth noting that a two-piece mollifier was used in [KRZ19].) In our table, we obtain 0.0632 unconditionally and 0.0854 on RSC. Using stronger spectral inputs on shifted convolution sums and a more extensive computer search, the best-known proportions for modular  $L$ -functions are 0.0696 unconditionally and 0.0896 on RSC ([AT21]).

## 7. GENERALIZATIONS AND FURTHER QUESTIONS

We sketch the general set-up. Let  $P \in C^1[0, 1]$  be a *given* real-valued function such that  $P(0) = 0$  and  $P(1) = 1$ , and we let

$$B := \int_0^1 P(x)^2 dx \quad \text{and} \quad C := \int_0^1 P'(x)^2 dx.$$

Let  $\beta \in \mathbb{R}$  and  $R > 0$  be constants at our disposal. By the same reasoning as in Section 3, we are readily led to the problem of optimizing the functional

$$K(S) := \int_0^R \left( e^t (c_0 S(t)^2 + c_1 S'(t)^2) + e^{-t} (c_0 (\beta - S(t))^2 + c_1 S'(t)^2) \right) dt, \quad (58)$$

with  $S \in C^1[0, R]$  and subject to boundary conditions

$$S(0) = \beta/2 \quad \text{and} \quad S(R) = \beta - 1, \quad (59)$$

where

$$c_0 := \frac{C}{\theta} - \theta B R^2 \quad \text{and} \quad c_1 := 4\theta B R^2.$$

For any  $S$  satisfying the constraints above and for any admissible value of  $\theta > 0$  (cf. (12)), we have

$$\kappa = 1 - \frac{1}{R} \log \left( \frac{1 + e^{2R}(\beta - 1)^2}{2} + c_1 \frac{e^R e^{R(1 - \beta)^2} - e^{-R}}{2} + \frac{e^R}{2R} K(S) \right). \quad (60)$$

Furthermore, for the optimal function  $S$ , we may simplify (58) as

$$K(S) = c_0 \beta^2 (1 - e^{-R}) - c_1 \beta S'(0) + 2(\beta - 1) c_1 S'(R) \cosh R - c_0 \beta \int_0^R e^{-t} S(t) dt. \quad (61)$$

**Remark 3.** The constant  $\beta$  arises from the constraint for (real-valued)  $Q \in C^1[0, 1]$ :

$$Q(0) = 1 \quad \text{and} \quad Q(y) + Q(1 - y) = \beta. \quad (62)$$

Again, we have  $S(-t) := \beta - S(t)$  for  $t \geq 0$  and  $Q(y) = S(2R(y - 1/2))$  for  $y \in [0, 1]$ .

We also let

$$c := -\frac{c_0}{c_1} = \frac{1}{4} - \frac{C}{4B\theta^2 R^2}.$$

With (59), the Euler–Lagrange equation for  $K(S)$  in this general case is given by

$$S''(t) + (\tanh t)S'(t) + cS(t) = \frac{c\beta}{1 + e^{2t}}. \quad (63)$$

**Remark 4.** The Euler–Lagrange equation above depends on  $R > 0$ ,  $\beta \in \mathbb{R}$ , and  $c < 1/4$  which further depends on  $B, C, \theta, R$ . When proving Theorem 1, the only parameter that varies is  $R$  (or equivalently,  $\theta$ ). In that case,  $c = -1$ ,  $\beta = 1$ ,  $B = 1/3$ , and  $C = 1$ .

Let  $\phi_c := (1 + \sqrt{1 - 4c})/2$ . A set of fundamental solutions to the homogeneous equation of (32) is given by

$$\begin{aligned} g_1(t; c) &:= \exp(tc/\phi_c) {}_2F_1(1/2, c/\phi_c; 1/2 - c/\phi_c; -e^{2t}), \\ g_2(t; c) &:= \exp(t\phi_c) {}_2F_1(1/2, \phi_c; 1/2 + \phi_c; -e^{2t}). \end{aligned} \quad (64)$$

Parallel to the notations in Section 3.1, we set

$$\begin{aligned} F^+(t; c) &:= {}_2F_1(1/2, \phi_c, 1/2 + \phi_c; -e^{2t}); \quad F^-(t; c) := {}_2F_1(1/2, c/\phi_c, 1/2 + c/\phi_c; -e^{2t}); \\ F_1^+(u; c) &:= {}_2F_1(1/2, 1 + \phi_c, 1/2 + \phi_c; -e^{2u}); \quad F_1^-(u; c) := {}_2F_1(3/2, c/\phi_c, 1/2 + c/\phi_c; -e^{2u}). \end{aligned}$$

The Wronskian for  $\{g_1(t; c), g_2(t; c)\}$  can be computed to be

$$\mathcal{W}(u; c) = \mathcal{W}(g_1, g_2)(u; c) = e^u(2\phi_c F^-(u; c)F_1^+(u; c) - F^+(u; c)F_1^-(u; c)). \quad (65)$$

Similar to before, we introduce:

$$f(t; c) = g_1(t; c) - \frac{g_1(0; c)}{g_2(0; c)} g_2(t; c), \quad g_0(t; c) = \frac{1}{2} \frac{g_2(t; c)}{g_2(0; c)}, \quad (66)$$

$$v_1(u; c) := \frac{g_2(u; c)}{\mathcal{W}(u; c)} \frac{1}{1 + e^{2u}}, \quad v_2(u; c) := -\frac{g_1(u; c)}{\mathcal{W}(u; c)} \frac{1}{1 + e^{2u}}. \quad (67)$$

It follows that the solution to the Euler–Lagrange equation is given by

$$S_R(t; c, \beta) = C_1(R; c, \beta)f(t; c) + \beta g_0(t; c) - c\beta g_1(t; c) \int_0^t v_1(u; c) du - c\beta g_2(t) \int_0^t v_2(u; c) du, \quad (68)$$

where

$$C_1(R; c, \beta) = \frac{\beta - 1 - \beta g_0(R; c) + c\beta g_1(R; c)w_1(R; c) + c\beta g_2(R; c)w_2(R; c)}{f(R; c)}. \quad (69)$$

We conclude this article with a few questions intended to stimulate future research.

(1) In [Con89], the following choice of  $P$  in the mollifier was used:

$$P(x) = P_r(x) := \frac{\sinh(rx)}{\sinh(r)}, \quad (70)$$

which was shown to be optimal. In this case, we have

$$B = \frac{\coth(r) - r\operatorname{csch}^2(r)}{2r} \quad \text{and} \quad C = \frac{r}{2} \operatorname{csch}(r)(\cosh(r) + r\operatorname{csch}(r)).$$



It is natural to ask what the largest possible value of  $\kappa = \kappa(\theta)$ , as given in (60), would be when combining (70) with our constructions (61) and (68). More precisely, for which choices of  $\beta$ ,  $r$ ,  $R$  optimize the value of  $\kappa$ ?

- (2) Study the optimization problem (58) *jointly* in the variables  $P$  and  $S$ . It is likely that  $P$  and  $S$  given in (70) and (68) satisfy the corresponding Euler–Lagrange equation.
- (3) Our optimal linear combination, together with the optimal (Levinson-type) mollifier, should give better values of  $\kappa$ . When  $\theta$  is large, say  $\theta = 4/7 - \epsilon$ , it is of interest to know how much improvement this would offer over [Con89].

We expect that the gain may be modest, likely not matching the state-of-the-art improvements achieved through more sophisticated mollifiers with multiple pieces, e.g., those developed in [BCY11], [Fen12] and [PR+20].

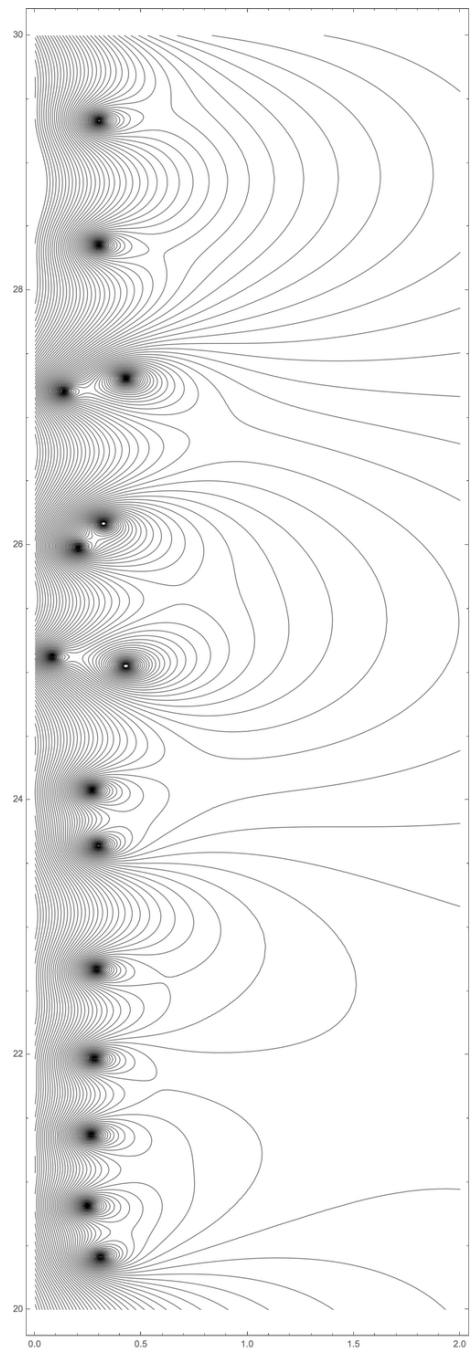
- (4) An interesting question is whether one can choose a simpler function  $Q$  to prove our Theorem 1, albeit at the expense of weaker numerical constants for  $\kappa$ .
- (5) Prove that  $\kappa(\theta) > 2\theta/3$  for any  $\theta \in (0, 1/2]$ , using  $P(x) = x$  and  $Q(y) = Q_R(y) = S_R(2R(y - 1/2))$  with  $S_R$  defined in (37).

It suffices to establish a good lower bound for  $C_1(R)$  for  $R \geq 2\sqrt{3/5}$ .

- (6) In view of Proposition 1, we wonder, how does the configuration of zeros for the function  $Q_R(-\frac{1}{L} \frac{d}{ds})\zeta(s)$  changes as  $R$  varies, where  $Q_R(y) = S_R(2R(y - 1/2))$  is the ‘optimal’ function determined in Section 3.1.

While  $Q_R(-\frac{1}{L} \frac{d}{ds})\zeta(s)$  serves as (pointwise) approximations to Siegel’s function  $f(s)$ , we suspect that, as  $R \rightarrow \infty$ , its zeros are pushed to the left relatively far from the critical line. This should stand in contrast to the distribution of zeros of  $f(s)$  (see [Con16, Fig. 5]), which appears to exhibit clusters of zeros near the critical line, both to its left and right.

Below is a contour plot of  $Q(-\frac{1}{L} \frac{d}{ds})\zeta(s)$ , where  $Q(y) = 0.492 + 0.602(1 - 2x) - 0.08(1 - 2x)^3 - 0.06(1 - 2x)^5 + 0.046(1 - 2x)^7$  is the polynomial used in [Con89].



APPENDIX A. MATHEMATICA COMMANDS (ODE\_CHECK.NB, PRE\_COMPUTE.NB, ASYMP.NB,  
INTEGRAL\_KAPPA.NB)

```
(*Verifying the ODE is satisfied*)

In[1]:= F+[t_, c_] := Hypergeometric2F1[ $\frac{1}{2}, \frac{1 + \sqrt{1 - 4c}}{2}, \frac{2 + \sqrt{1 - 4c}}{2}, -e^{2t}$ ]
In[2]:= F-[t_, c_] := Hypergeometric2F1[ $\frac{1}{2}, \frac{1 - \sqrt{1 - 4c}}{2}, \frac{2 - \sqrt{1 - 4c}}{2}, -e^{2t}$ ]
In[3]:= F1+[t_, c_] := Hypergeometric2F1[ $\frac{1}{2}, \frac{3 + \sqrt{1 - 4c}}{2}, \frac{2 + \sqrt{1 - 4c}}{2}, -e^{2t}$ ]
In[4]:= F1-[t_, c_] := Hypergeometric2F1[ $\frac{3}{2}, \frac{1 - \sqrt{1 - 4c}}{2}, \frac{2 - \sqrt{1 - 4c}}{2}, -e^{2t}$ ]
In[5]:= g1[t_, c_] := Exp[(1 -  $\sqrt{1 - 4c}$ ) * t / 2] * F-[t, c]
In[6]:= g2[t_, c_] := Exp[(1 +  $\sqrt{1 - 4c}$ ) * t / 2] * F+[t, c]
In[7]:= f[t_, c_] := g1[t, c] - (F-[0, c] / F+[0, c]) * g2[t, c]
In[8]:= g0[t_, c_] := g2[t, c] / (2 * F+[0, c])
In[9]:= W[u_, c_] := Exp[u] * ((1 +  $\sqrt{1 - 4c}$ ) F-[u, c] F1+[u, c] - F+[u, c] F1-[u, c])
In[10]:= v1[u_, c_] := g2[u, c] / (W[u, c] * (1 + Exp[2 u]))
In[11]:= v2[u_, c_] := -g1[u, c] / (W[u, c] * (1 + Exp[2 u]))
In[12]:= FullSimplify[D[g1[t, c], {t, 2}] + Tanh[t] * D[g1[t, c], {t, 1}] + c * g1[t, c]]
Out[12]=
0

In[14]:= FullSimplify[D[g2[t, c], {t, 2}] + Tanh[t] * D[g2[t, c], {t, 1}] + c * g2[t, c]]
Out[14]=
0

In[15]:= FullSimplify[Expand[Wronskian[{g1[t, c], g2[t, c]}, t] - W[t, c]]]
Out[15]=
0

In[16]:= P3 = D[g1[t, c] * Integrate[v1[u, c], {u, 0, t}], {t, 2}] +
      Tanh[t] * D[g1[t, c] * Integrate[v1[u, c], {u, 0, t}], {t, 1}] -
      g1[t, c] * Integrate[v1[u, c], {u, 0, t}];
In[17]:= P4 = D[g2[t, c] * Integrate[v2[u, c], {u, 0, t}], {t, 2}] +
      Tanh[t] * D[g2[t, c] * Integrate[v2[u, c], {u, 0, t}], {t, 1}] -
      g2[t, c] * Integrate[v2[u, c], {u, 0, t}];
In[20]:= FullSimplify[(P3 /. c -> -1) + (P4 /. c -> -1)]
Out[20]=

$$-\frac{1}{1 + e^{2t}}$$

```

```

(*Set-up and Pre-compute vi[u], wj[t], C-1[R]*)
In[1]:= T[a_, b_, c_, x_] := (-x) ^ (-a) / Gamma[b] / Gamma[c - a] / Gamma[a - b + 1]
Hypergeometric2F1[a, a - c + 1, a - b + 1, 1 / x] * Pi Gamma[c] / Sin[Pi (b - a)] -
(-x) ^ (-b) / Gamma[a] / Gamma[c - b] / Gamma[b - a + 1]
Hypergeometric2F1[b, b - c + 1, b - a + 1, 1 / x] * Pi * Gamma[c] / Sin[Pi (b - a)]

In[2]:= F+[t_] := T[1 / 2, (1 + Sqrt[5]) / 2, (2 + Sqrt[5]) / 2, -Exp[2 t]]
In[3]:= F-[t_] := T[1 / 2, (1 - Sqrt[5]) / 2, (2 - Sqrt[5]) / 2, -Exp[2 t]]
In[4]:= F1+[t_] := T[1 / 2, (3 + Sqrt[5]) / 2, (2 + Sqrt[5]) / 2, -Exp[2 t]]
In[5]:= F1-[t_] := T[3 / 2, (1 - Sqrt[5]) / 2, (2 - Sqrt[5]) / 2, -Exp[2 t]]
In[6]:= g1[t_] := Exp[(1 - Sqrt[5]) * t / 2] * F-[t]
In[7]:= g2[t_] := Exp[(1 + Sqrt[5]) * t / 2] * F+[t]
In[8]:= f[t_] := g1[t] - (F-[0] / F+[0]) * g2[t]
In[9]:= g0[t_] := g2[t] / (2 * F+[0])
In[10]:= W[u_] := Exp[u] * ((1 + Sqrt[5]) F-[u] F1+[u] - F+[u] F1-[u])
In[11]:= v1[u_] := g2[u] / (W[u] * (1 + Exp[2 u]))
In[12]:= v2[u_] := -g1[u] / (W[u] * (1 + Exp[2 u]))
In[13]:= vv1[u_] := - 
$$\left( \left( 2 \left( e^{2u} \right)^{\frac{5}{4} - \frac{\sqrt{5}}{4}} \cos \left[ \frac{\sqrt{5}}{2} \pi \right]^2 \text{Gamma} \left[ -\frac{\sqrt{5}}{2} \right] \text{Gamma} \left[ \frac{1}{2} - \frac{\sqrt{5}}{2} \right]^2 \text{Gamma} \left[ 2 + \frac{\sqrt{5}}{2} \right] \right. \right. \\ \left. \left. \frac{\left( e^{2u} \right)^{\frac{\sqrt{5}}{2}} \pi \text{Gamma} \left[ 1 + \frac{\sqrt{5}}{2} \right] \text{Hypergeometric2F1} \left[ \frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), 1 - \frac{\sqrt{5}}{2}, -e^{-2u} \right]}{\text{Gamma} \left[ 1 - \frac{\sqrt{5}}{2} \right]} - \right. \right. \\ \left. \left. \text{Gamma} \left[ \frac{1}{2} (1 + \sqrt{5}) \right]^2 \right. \right. \\ \left. \left. \text{Hypergeometric2F1} \left[ \frac{1}{2}, \frac{1}{2} (1 + \sqrt{5}), \frac{1}{2} (2 + \sqrt{5}), -e^{-2u} \right] \right) \right) / \\ \left( (1 + e^{2u}) \pi^3 \left( (5 + 2 \sqrt{5}) e^{2u} \text{Hypergeometric2F1} \left[ \frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), -\frac{\sqrt{5}}{2}, -e^{-2u} \right] \right. \right. \\ \left. \left. \text{Hypergeometric2F1} \left[ \frac{1}{2}, \frac{1}{2} (1 + \sqrt{5}), \frac{1}{2} (2 + \sqrt{5}), -e^{-2u} \right] - \right. \right. \\ \left. \left. (1 + \sqrt{5}) \text{Hypergeometric2F1} \left[ \frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), 1 - \frac{\sqrt{5}}{2}, -e^{-2u} \right] \right. \right. \\ \left. \left. \left. \text{Hypergeometric2F1} \left[ \frac{3}{2}, \frac{1}{2} (3 + \sqrt{5}), \frac{1}{2} (4 + \sqrt{5}), -e^{-2u} \right] \right) \right) \right)$$


```

$$\begin{aligned}
\text{In[14]:= } vv2[u_] := & \left( (e^{2u})^{\frac{5}{4} - \frac{\sqrt{5}}{4}} (1 + \cos[\sqrt{5} \pi]) \Gamma\left[-\frac{\sqrt{5}}{2}\right] \right. \\
& \Gamma\left[2 + \frac{\sqrt{5}}{2}\right] \Gamma\left[\frac{1}{2} (1 + \sqrt{5})\right]^2 \left( (e^{2u})^{\frac{\sqrt{5}}{2}} \Gamma\left[\frac{1}{2} - \frac{\sqrt{5}}{2}\right]^2 \right. \\
& \Gamma\left[1 + \frac{\sqrt{5}}{2}\right] \text{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), 1 - \frac{\sqrt{5}}{2}, -e^{-2u}\right] - \\
& \left. \pi \Gamma\left[1 - \frac{\sqrt{5}}{2}\right] \text{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 + \sqrt{5}), \frac{1}{2} (2 + \sqrt{5}), -e^{-2u}\right] \right) \Bigg) / \\
& \left( (1 + e^{2u}) \pi^3 \Gamma\left[1 + \frac{\sqrt{5}}{2}\right] \left( (5 + 2\sqrt{5}) e^{2u} \text{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), \right. \right. \right. \\
& \left. \left. -\frac{\sqrt{5}}{2}, -e^{-2u}\right] \text{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 + \sqrt{5}), \frac{1}{2} (2 + \sqrt{5}), -e^{-2u}\right] - \right. \\
& \left. (1 + \sqrt{5}) \text{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), 1 - \frac{\sqrt{5}}{2}, -e^{-2u}\right] \right. \\
& \left. \left. \text{Hypergeometric2F1}\left[\frac{3}{2}, \frac{1}{2} (3 + \sqrt{5}), \frac{1}{2} (4 + \sqrt{5}), -e^{-2u}\right] \right) \right)
\end{aligned}$$

In[15]:= Simplify[PowerExpand[Cancel[FullSimplify[v1[u]] / vv1[u]]]]

Out[15]=  
1

In[16]:= Simplify[PowerExpand[Cancel[FullSimplify[v2[u]] / vv2[u]]]]

Out[16]=  
1

In[17]:= Tbv1[t\_, r\_] := Table[N[vv1[u], 15], {u, 0, t, r}]

In[18]:= Tbv140 = Tbv1[40, 1 / 5000];

Export["Tbv140oneOver5000.mx", Tbv140]

In[19]:= Tbv2[t\_, r\_] := Table[N[vv2[u], 15], {u, 0, t, r}]

In[20]:= Tbv240 = Tbv2[40, 1 / 5000];

Export["Tbv240oneOver5000.mx", Tbv240]

In[21]:= ww1[t\_] :=

Total[Flatten[Select[Transpose[{Range[0, 40, 1 / 5000], Tbv140}], #[[1]] ≤ t &]][  
2 ;; ;; 2]]] \* 1 / 5000

In[22]:= Tbw1t40ref = Table[ww1[t], {t, 0, 40, 1 / 100}];

Export["Tbw1t40ref1over100.mx", Tbw1t40ref]

In[23]:= ww2[t\_] :=

Total[Flatten[Select[Transpose[{Range[0, 40, 1 / 5000], Tbv240}], #[[1]] ≤ t &]][  
2 ;; ;; 2]]] \* 1 / 5000

In[24]:= Tbw2t40ref = Table[ww2[t], {t, 0, 40, 1 / 100}];

```

Export["Tbww2t40ref10over100.mx", Tbww2t40ref]

(*D0, N1, N2, N3 are determined in the "Asymptotic" file.*)

In[25]:= D0 = -2 Hypergeometric2F1[ $\frac{1}{2}, \frac{1}{2} (1 + \sqrt{5})$ ,  $\frac{1}{2} (2 + \sqrt{5})$ , -1];

In[26]:= N1 = - $\frac{1}{\sqrt{5} \pi^2}$  4 Cos[ $\frac{\sqrt{5} \pi}{2}$ ] Cot[ $\frac{\sqrt{5} \pi}{2}$ ] Gamma[ $\frac{1}{2} - \frac{\sqrt{5}}{2}$ ]2
Gamma[ $1 + \frac{\sqrt{5}}{2}$ ]2 Hypergeometric2F1[ $\frac{1}{2}, \frac{1}{2} (1 - \sqrt{5})$ ,  $1 - \frac{\sqrt{5}}{2}$ , -1] +
 $\frac{1}{\sqrt{5} \pi^3}$  4 Cos[ $\frac{\sqrt{5} \pi}{2}$ ] Cot[ $\frac{\sqrt{5} \pi}{2}$ ] Gamma[ $\frac{1}{2} - \frac{\sqrt{5}}{2}$ ]2 Gamma[ $1 - \frac{\sqrt{5}}{2}$ ] Gamma[ $1 + \frac{\sqrt{5}}{2}$ ]
Gamma[ $\frac{1}{2} (1 + \sqrt{5})$ ]2 Hypergeometric2F1[ $\frac{1}{2}, \frac{1}{2} (1 + \sqrt{5})$ ,  $\frac{1}{2} (2 + \sqrt{5})$ , -1];

In[27]:= N2 = - $\frac{\pi \text{Csc}[\frac{\sqrt{5} \pi}{2}] \text{Gamma}[1 + \frac{\sqrt{5}}{2}]}{\text{Gamma}[1 - \frac{\sqrt{5}}{2}] \text{Gamma}[\frac{1}{2} (1 + \sqrt{5})]^2}$ ;

In[28]:= N3 = - $\frac{2 \pi^2 \text{Csc}[\frac{\sqrt{5} \pi}{2}]^2 \text{Gamma}[1 + \frac{\sqrt{5}}{2}]^2 \text{Hypergeometric2F1}[\frac{1}{2}, \frac{1}{2} (1 - \sqrt{5})$ ,  $1 - \frac{\sqrt{5}}{2}$ , -1]}{\text{Gamma}[1 - \frac{\sqrt{5}}{2}]^2 \text{Gamma}[\frac{1}{2} (1 + \sqrt{5})]^4} +
 $\left( 2 \pi \text{Csc}[\frac{\sqrt{5} \pi}{2}]^2 \text{Gamma}[1 + \frac{\sqrt{5}}{2}] \text{Hypergeometric2F1}[\frac{1}{2}, \frac{1}{2} (1 + \sqrt{5})$ ,  $\frac{1}{2} (2 + \sqrt{5})$ , -1]  $\right) / \left( \text{Gamma}[1 - \frac{\sqrt{5}}{2}] \text{Gamma}[\frac{1}{2} (1 + \sqrt{5})]^2 \right)$ ;

In[34]:= cLim = N[(N1 * Tbww1t40ref[[-1]] + N2 + N3 * Tbww2t40ref[[-1]]) / D0, 15];

In[35]:= Sinfdata = cLim * Table[N[f[t], 15], {t, 0, 40, 1/100}] +
Table[N[g0[t], 15], {t, 0, 40, 1/100}] +
Table[N[g1[t], 15], {t, 0, 40, 1/100}] * Tbww1t40ref +
Table[N[g2[t], 15], {t, 0, 40, 1/100}] * Tbww2t40ref;

Export["Sinf40oneOver100.mx", Sinfdata];

In[36]:= ConstCnum =
-2 * Table[N[F-[R], 15], {R, 0, 40, 1/100}] * N[F+[0], 15] * Tbww1t40ref -
Table[N[Exp[Sqrt[5] * R] * F+[R], 15], {R, 0, 40, 1/100}] - 2 * N[F+[0], 15] *
Table[N[Exp[Sqrt[5] * R] * F+[R], 15], {R, 0, 40, 1/100}] * Tbww2t40ref;

In[37]:= ConstCdenom = 2 * N[F+[0], 15] * Table[N[F-[R], 15], {R, 0, 40, 1/100}] -
2 * N[F-[0], 15] * Table[N[Exp[Sqrt[5] * R] * F+[R], 15], {R, 0, 40, 1/100}];

In[38]:= TbConstC = ConstCnum / ConstCdenom;

Export["ConstC40oneOver100.mx", TbConstC];

(*Consistency check for integrals of v1[u], v2[u], and value of C1[R]*)

```

```

In[39]:= c1[R_] := (-2 * F^-[R] * F+[0] * NIntegrate[vv1[u], {u, 0, R}] -
      Exp[Sqrt[5] * R] * F+[R] (1 + 2 * F+[0] * NIntegrate[vv2[u], {u, 0, R}])) /
      (2 * F^-[R] * F+[0] - 2 * Exp[Sqrt[5] * R] * F^-[0] * F+[R])

In[41]:= TBNIntvv1 = Table[NIntegrate[vv1[u], {u, 0, t}], {t, 0, 40, 1/100}];

In[45]:= Count[Abs[TBNIntvv1 - Tbww1t40ref], x_ /; x < 10^-4]
Out[45]=
4001

In[47]:= Length[TBNIntvv1]
Out[47]=
4001

In[48]:= TBNIntvv2 = Table[NIntegrate[vv2[u], {u, 0, t}], {t, 0, 40, 1/100}];

In[52]:= Count[Abs[TBNIntvv2 - Tbww2t40ref], x_ /; x < 2 * 10^-4]
Out[52]=
4001

In[56]:= NIntegrate[vv1[u], {u, 0, 40}]
Out[56]=
1.32084

In[57]:= Tbww1t40ref[[-1]]
Out[57]=
1.32087512814678

In[58]:= NIntegrate[vv2[u], {u, 0, 40}]
Out[58]=
2.81665

In[59]:= Tbww2t40ref[[-1]]
Out[59]=
2.81669456818713

In[60]:= cLim
Out[60]=
0.67408914132169

In[61]:= TBNConstC = Table[c1[R], {R, 0, 40, 1/100}];

In[63]:= Count[Abs[TBNConstC - TbConstC], x_ /; x < 10^-4]
Out[63]=
4000

In[64]:= TbConstC[[-1]]
Out[64]=
0.6740891413217

In[65]:= c1[40]
Out[65]=
0.674123

```

```

(*Mathematica code for the asymptotics of the components of S_{R}(t)*)

(*T[a_,b_,c_,x_], F+[t_], F-[t_], F1+[t_],
F1-[t_], f[t_], g0[t_], g1[t_], g2[t_] as before! *)

In[10]:= G[u_] := (1 + Exp[2 u]) * ((1 + Sqrt[5]) F-[u] F1+[u] - F+[u] F1-[u])

In[11]:= v1[u_] := (Exp[(Sqrt[5] - 1) * u / 2] * F+[u]) / G[u]

In[12]:= v2[u_] := -Exp[(-Sqrt[5] - 1) * u / 2] * F-[u] / G[u]

In[13]:= Expand[N[FullSimplify[Series[F+[t], {t, Infinity, 0}]], 9]]
Out[13]=
0.66377719 × 2.71828183-7.23606798 t+0[ $\frac{1}{t}$ ]2 - 1.05406313 × 2.71828183-5.23606798 t+0[ $\frac{1}{t}$ ]2 +
1.05684133 × 2.71828183-5.00000000 t+0[ $\frac{1}{t}$ ]2 + 2.75957310 × 2.71828183-3.23606798 t+0[ $\frac{1}{t}$ ]2 -
3.25368611 × 2.71828183-3.00000000 t+0[ $\frac{1}{t}$ ]2 + 1.24279751 × 2.71828183-t+0[ $\frac{1}{t}$ ]2

In[14]:= Expand[N[FullSimplify[Series[F-[t], {t, Infinity, 0}]], 9]]
Out[14]=
-1.28034171 × 2.71828183-5.00000000 t+0[ $\frac{1}{t}$ ]2 + 2.03315363 × 2.71828183-3.00000000 t+0[ $\frac{1}{t}$ ]2 -
2.34666620 × 2.71828183-2.76393202 t+0[ $\frac{1}{t}$ ]2 - 5.3228653 × 2.71828183-t+0[ $\frac{1}{t}$ ]2 +
7.2246562 × 2.71828183-0.76393202 t+0[ $\frac{1}{t}$ ]2 - 2.75957310 × 2.718281831.23606798 t+0[ $\frac{1}{t}$ ]2

In[15]:= Expand[N[FullSimplify[Series[f[t], {t, Infinity, 0}]], 9]]
Out[15]=
-0.34055508 × 2.71828183-5.61803399 t+0[ $\frac{1}{t}$ ]2 + 0.54079375 × 2.71828183-3.61803399 t+0[ $\frac{1}{t}$ ]2 -
0.85037291 × 2.71828183-3.38196601 t+0[ $\frac{1}{t}$ ]2 - 1.41581641 × 2.71828183-1.61803399 t+0[ $\frac{1}{t}$ ]2 +
2.61803399 × 2.71828183-1.38196601 t+0[ $\frac{1}{t}$ ]2 - 1.00000000 × 2.718281830.618033989 t+0[ $\frac{1}{t}$ ]2

In[16]:= Expand[N[FullSimplify[Series[g0[t], {t, Infinity, 0}]], 9]]
Out[16]=
0.43719207 × 2.71828183-5.61803399 t+0[ $\frac{1}{t}$ ]2 - 0.69425110 × 2.71828183-3.61803399 t+0[ $\frac{1}{t}$ ]2 +
0.69608094 × 2.71828183-3.38196601 t+0[ $\frac{1}{t}$ ]2 + 1.81757297 × 2.71828183-1.61803399 t+0[ $\frac{1}{t}$ ]2 -
2.14301695 × 2.71828183-1.38196601 t+0[ $\frac{1}{t}$ ]2 + 0.81855964 × 2.718281830.618033989 t+0[ $\frac{1}{t}$ ]2

In[17]:= Expand[N[FullSimplify[Series[g1[t], {t, Infinity, 0}]], 9]]
Out[17]=
-1.28034171 × 2.71828183-5.61803399 t+0[ $\frac{1}{t}$ ]2 + 2.03315363 × 2.71828183-3.61803399 t+0[ $\frac{1}{t}$ ]2 -
2.34666620 × 2.71828183-3.38196601 t+0[ $\frac{1}{t}$ ]2 - 5.3228653 × 2.71828183-1.61803399 t+0[ $\frac{1}{t}$ ]2 +
7.2246562 × 2.71828183-1.38196601 t+0[ $\frac{1}{t}$ ]2 - 2.75957310 × 2.718281830.618033989 t+0[ $\frac{1}{t}$ ]2

In[18]:= Expand[N[FullSimplify[Series[g2[t], {t, Infinity, 0}]], 9]]
Out[18]=
0.66377719 × 2.71828183-5.61803399 t+0[ $\frac{1}{t}$ ]2 - 1.05406313 × 2.71828183-3.61803399 t+0[ $\frac{1}{t}$ ]2 +
1.05684133 × 2.71828183-3.38196601 t+0[ $\frac{1}{t}$ ]2 + 2.75957310 × 2.71828183-1.61803399 t+0[ $\frac{1}{t}$ ]2 -
3.25368611 × 2.71828183-1.38196601 t+0[ $\frac{1}{t}$ ]2 + 1.24279751 × 2.718281830.618033989 t+0[ $\frac{1}{t}$ ]2

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```

In[19]:= Expand[N[FullSimplify[Series[F1+[u], {u, Infinity, 0}]], 9]]
Out[19]=

$$0.90106767 \times 2.71828183^{-9.23606798 u+0 \left[\frac{1}{u}\right]^2} - 0.82047372 \times 2.71828183^{-7.23606798 u+0 \left[\frac{1}{u}\right]^2} +$$


$$0.65144684 \times 2.71828183^{-5.23606798 u+0 \left[\frac{1}{u}\right]^2} - 0.57606832 \times 2.71828183^{-3.23606798 u+0 \left[\frac{1}{u}\right]^2} -$$


$$0.237353203 \times 2.71828183^{-1.23606798 u+0 \left[\frac{1}{u}\right]^2} + 0.85875196 \times 2.71828183^{-u+0 \left[\frac{1}{u}\right]^2}$$


In[20]:= Expand[N[FullSimplify[Series[F1-[u], {u, Infinity, 0}]], 9]]
Out[20]=

$$-5.6244313 \times 2.71828183^{-7.00000000 u+0 \left[\frac{1}{u}\right]^2} + 5.1213668 \times 2.71828183^{-5.00000000 u+0 \left[\frac{1}{u}\right]^2} -$$


$$4.0663073 \times 2.71828183^{-3.00000000 u+0 \left[\frac{1}{u}\right]^2} + 4.1393597 \times 2.71828183^{-1.00000000 u+0 \left[\frac{1}{u}\right]^2} +$$


$$1.70550997 \times 2.71828183^{-u+0 \left[\frac{1}{u}\right]^2} - 6.1705930 \times 2.71828183^{1.23606798 u+0 \left[\frac{1}{u}\right]^2}$$


In[21]:= Expand[FullSimplify[Series[G[u], {u, Infinity, 0}]]]
Out[21]=

$$-\frac{1}{44 (37 + \sqrt{5})}$$


$$\left( 1350 e^{-12 u+0 \left[\frac{1}{u}\right]^2} + 90 \sqrt{5} e^{-12 u+0 \left[\frac{1}{u}\right]^2} - 1995 e^{-10 u+0 \left[\frac{1}{u}\right]^2} - 903 \sqrt{5} e^{-10 u+0 \left[\frac{1}{u}\right]^2} + 225 e^{-8 u+0 \left[\frac{1}{u}\right]^2} + \right.$$


$$\left. 345 \sqrt{5} e^{-8 u+0 \left[\frac{1}{u}\right]^2} + 3350 e^{-6 u+0 \left[\frac{1}{u}\right]^2} - 290 \sqrt{5} e^{-6 u+0 \left[\frac{1}{u}\right]^2} \right) + \left( \frac{5 + 37 \sqrt{5}}{37 + \sqrt{5}} + 0 \left[ \frac{1}{u} \right]^1 \right)$$


In[22]:= (*For v_1[u] ...*)
In[23]:= Expand[N[FullSimplify[
Series[(Exp[(Sqrt[5] - 1) * u / 2] * F+[u]) / Sqrt[5], {u, Infinity, 0}]], 9]]
Out[23]=

$$0.296850182 \times 2.71828183^{-6.61803399 u+0 \left[\frac{1}{u}\right]^2} - 0.471391363 \times 2.71828183^{-4.61803399 u+0 \left[\frac{1}{u}\right]^2} +$$


$$0.47263381 \times 2.71828183^{-2.61803399 u+0 \left[\frac{1}{u}\right]^2} + 1.23411861 \times 2.71828183^{-0.61803399 u+0 \left[\frac{1}{u}\right]^2} -$$


$$1.45509266 \times 2.71828183^{-0.38196601 u+0 \left[\frac{1}{u}\right]^2} + 0.55579594 \times 2.71828183^{0.38196601 u+0 \left[\frac{1}{u}\right]^2}$$


In[24]:= (*For v_2[u] ...*)
In[25]:= Expand[N[FullSimplify[
Series[-Exp[(-Sqrt[5] - 1) * u / 2] * F-[u] / Sqrt[5], {u, Infinity, 0}]], 9]]
Out[25]=

$$0.57258622 \times 2.71828183^{-6.61803399 u+0 \left[\frac{1}{u}\right]^2} - 0.90925394 \times 2.71828183^{-4.61803399 u+0 \left[\frac{1}{u}\right]^2} +$$


$$1.04946103 \times 2.71828183^{-2.61803399 u+0 \left[\frac{1}{u}\right]^2} + 2.38045773 \times 2.71828183^{-0.61803399 u+0 \left[\frac{1}{u}\right]^2} -$$


$$3.23096447 \times 2.71828183^{-0.38196601 u+0 \left[\frac{1}{u}\right]^2} + 1.23411861 \times 2.71828183^{0.38196601 u+0 \left[\frac{1}{u}\right]^2}$$


In[26]:= (*The asymptotic for the denominator of C_1[R]...*)
In[27]:= Expand[FullSimplify[Series[
(2 * F-[R] * F+[0] - 2 * Exp[Sqrt[5] * R] * F-[0] * F+[R]), {R, Infinity, 0}]]];

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In[28]:= N[Expand[FullSimplify[Series[
      (2 * F-[R] * F+[0] - 2 * Exp[Sqrt[5] * R] * F-[0] * F+[R]), {R, Infinity, 0}]]]]]
Out[28]=
-0.517056 × 2.71828-5. R+0[1/R]2 + 0.821073 × 2.71828-3. R+0[1/R]2 -
1.2911 × 2.71828-2.76393 R+0[1/R]2 - 2.1496 × 2.71828-R+0[1/R]2 +
3.97489 × 2.71828-0.763932 R+0[1/R]2 - 1.51827 × 2.718281.23607 R+0[1/R]2

In[29]:= (*So, the denominator is of order Exp[(Sqrt[5]-1)R] with coefficient -1.5182 *)
In[30]:= D0 = -2 Hypergeometric2F1[1/2, 1/2 (1 + Sqrt[5]), 1/2 (2 + Sqrt[5]), -1];
In[31]:= (*The asymptotic for the numerator of C_1[R]...consists of 3 terms*)
(*Firstly...*)
In[32]:= Expand[FullSimplify[Series[-2 * F-[R] * F+[0], {R, Infinity, 0}]]];
In[33]:= N[Expand[FullSimplify[Series[-2 * F-[R] * F+[0], {R, Infinity, 0}]]]]]
Out[33]=
1.94391 × 2.71828-5. R+0[1/R]2 - 3.08688 × 2.71828-3. R+0[1/R]2 + 3.56288 × 2.71828-2.76393 R+0[1/R]2 +
8.08157 × 2.71828-R+0[1/R]2 - 10.969 × 2.71828-0.763932 R+0[1/R]2 + 4.18979 × 2.718281.23607 R+0[1/R]2

In[34]:= N1 = - 1/√5 4 Cos[√5 π/2] Cot[√5 π/2] Gamma[1/2 - √5/2]2
Gamma[1 + √5/2]2 Hypergeometric2F1[1/2, 1/2 (1 - √5), 1 - √5/2, -1] +
1/√5 4 Cos[√5 π/2] Cot[√5 π/2] Gamma[1/2 - √5/2]2 Gamma[1 - √5/2] Gamma[1 + √5/2]
Gamma[1/2 (1 + √5)]2 Hypergeometric2F1[1/2, 1/2 (1 + √5), 1/2 (2 + √5), -1];

In[35]:= N[N1]
Out[35]=
4.18979

In[36]:= (*Secondly, ...*)
In[37]:= Expand[FullSimplify[Series[- Exp[Sqrt[5] * R] * F+[R], {R, Infinity, 0}]]];
In[38]:= N[Expand[FullSimplify[Series[- Exp[Sqrt[5] * R] * F+[R], {R, Infinity, 0}]]]]]
Out[38]=
-0.663777 × 2.71828-5. R+0[1/R]2 + 1.05406 × 2.71828-3. R+0[1/R]2 -
1.05684 × 2.71828-2.76393 R+0[1/R]2 - 2.75957 × 2.71828-R+0[1/R]2 +
3.25369 × 2.71828-0.763932 R+0[1/R]2 - 1.2428 × 2.718281.23607 R+0[1/R]2

In[39]:= N2 = - π Csc[√5 π/2] Gamma[1 + √5/2]
Gamma[1 - √5/2] Gamma[1/2 (1 + √5)]2;

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In[40]:= N[N2]
Out[40]=
-1.2428

In[41]:= (*Thirdly,...*)

In[42]:= Expand[
FullSimplify[ Series[- Exp[Sqrt[5] * R] * F*[R] (2 * F*[0]), {R, Infinity, 0}]]];

In[43]:= N[Expand[
FullSimplify[ Series[- Exp[Sqrt[5] * R] * F*[R] (2 * F*[0]), {R, Infinity, 0}]]]]
Out[43]=
-1.0078 * 2.71828-5. R+0 $\left[\frac{1}{R}\right]^2$  + 1.60036 * 2.71828-3. R+0 $\left[\frac{1}{R}\right]^2$  - 1.60457 * 2.71828-2.76393 R+0 $\left[\frac{1}{R}\right]^2$  -
4.18979 * 2.71828-R+0 $\left[\frac{1}{R}\right]^2$  + 4.93999 * 2.71828-0.763932 R+0 $\left[\frac{1}{R}\right]^2$  - 1.88691 * 2.718281.23607 R+0 $\left[\frac{1}{R}\right]^2$ 

In[44]:= N3 = - 
$$\frac{2 \pi^2 \operatorname{Csc}\left[\frac{\sqrt{5} \pi}{2}\right]^2 \operatorname{Gamma}\left[1 + \frac{\sqrt{5}}{2}\right]^2 \operatorname{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 - \sqrt{5}), 1 - \frac{\sqrt{5}}{2}, -1\right]}{\operatorname{Gamma}\left[1 - \frac{\sqrt{5}}{2}\right]^2 \operatorname{Gamma}\left[\frac{1}{2} (1 + \sqrt{5})\right]^4} +$$


$$\left(2 \pi \operatorname{Csc}\left[\frac{\sqrt{5} \pi}{2}\right]^2 \operatorname{Gamma}\left[1 + \frac{\sqrt{5}}{2}\right] \operatorname{Hypergeometric2F1}\left[\frac{1}{2}, \frac{1}{2} (1 + \sqrt{5}), \frac{1}{2} (2 + \sqrt{5}), -1\right]\right) / \left(\operatorname{Gamma}\left[1 - \frac{\sqrt{5}}{2}\right] \operatorname{Gamma}\left[\frac{1}{2} (1 + \sqrt{5})\right]^2\right);$$


In[45]:= N[N3]
Out[45]=
-1.88691

In[46]:= (*Conclusion: C_1[R] is asymptotic to (N1*w1[Infinity]+N2+N3*w2[Infinity])/D0*)

```

```

In[*]:= (*Computing integrals for Theorem 1*)

(*T[a_,b_,c_,x_], F+[t_], F-[t_], F1+[t_], F1-[t_], f[t_], g0[t_],
g1[t_], g2[t_], v1[u_], v2[u_], vv1[u_], vv2[u_] as before! *)

In[15]:= SetDirectory[NotebookDirectory[]];

In[16]:= TbConstC = Import["ConstC40oneOver100.mx"];

In[17]:= c1[R_] := (-2 * F-[R] * F+[0] * NIntegrate[vv1[u], {u, 0, R}] -
Exp[Sqrt[5] * R] * F+[R] (1 + 2 * F+[0] * NIntegrate[vv2[u], {u, 0, R}]) ) /
(2 * F-[R] * F+[0] - 2 * Exp[Sqrt[5] * R] * F-[0] * F+[R])

In[18]:= Intexpf = NIntegrate[Exp[-t] * f[t], {t, 0, 40}]
Out[18]=
-2.11661

In[19]:= Intexpg0 = NIntegrate[Exp[-t] * g0[t], {t, 0, 80}]
Out[19]=
1.9453

In[20]:= Auxw1[t_?NumericQ] := NIntegrate[vv1[u], {u, 0, t}]

In[21]:= Intexpg1v1 = NIntegrate[Exp[-t] * g1[t] * Auxw1[t], {t, 0, 80}]
Out[21]=
-4.29439

In[22]:= Auxw2[t_?NumericQ] := NIntegrate[vv2[u], {u, 0, t}]

In[23]:= Intexpg2v2 = NIntegrate[Exp[-t] * g2[t] * Auxw2[t], {t, 0, 80}]
Out[23]=
4.02455

In[24]:= Sum3Int = Intexpg0 + Intexpg1v1 + Intexpg2v2
Out[24]=
1.67545

In[25]:= IntLimexpSRt = Intexpf * TbConstC[[-1]] + Sum3Int
Out[25]=
0.248666

In[26]:= fd0 = N[D[f[t], t] /. {t -> 0}, 15]
Out[26]=
-1.47277008628940

In[27]:= N[D[g0[t], t] /. {t -> 0}, 15]
Out[27]=
0.602775072614097

In[28]:= N[g1[0], 15]
Out[28]=
-1.07479835721849

In[29]:= N[g2[0], 15]
Out[29]=
0.759136812431294

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```

In[30]:= N[v1[0], 15]
Out[30]=
0.339496303363776

In[31]:= N[v2[0], 15]
Out[31]=
0.480664437769128

In[32]:= SLimder0 = TbConstC[[-1]] * N[D[f[t], t] /. {t -> 0}, 15] + N[D[g0[t], t] /. {t -> 0}, 15] +
N[g1[0], 15] * N[v1[0], 15] + N[g2[0], 15] * N[v2[0], 15]
Out[32]=
-0.3900032502170

In[33]:= Sum3Der = N[D[g0[t], t] /. {t -> 0}, 15] +
N[g1[0], 15] * N[v1[0], 15] + N[g2[0], 15] * N[v2[0], 15]
Out[33]=
0.60277507261410

In[34]:= 1 - SLimder0 - IntLimexpSRt
Out[34]=
1.14134

In[35]:= 1 - (fd0 * x + Sum3Der) - (Intexpf * x + Sum3Int)
Out[35]=
-1.27823 + 3.58938 x

In[36]:= Kappa[Th_] := 1 - (Sqrt[3 / 5] / Th) ^ (-1) *
Log[1 / 2 - 1 / Sqrt[15] + (2 / Sqrt[15]) * Exp[Sqrt[3 / 5] / Th] *
(1 - Exp[-Sqrt[3 / 5] / Th] - (fd0 * c1[Sqrt[3 / 5] / Th] + Sum3Der) -
(Intexpf * c1[Sqrt[3 / 5] / Th] + Sum3Int))]
In[37]:= Kappa[2 / 3]
Out[37]=
0.36477

In[38]:= Kappa[1 / 2]
Out[38]=
0.334112

In[39]:= Kappa[1 / 4]
Out[39]=
0.176131

In[40]:= Kappa[1 / 6]
Out[40]=
0.114663

In[41]:= Kappa[1 / 8]
Out[41]=
0.0854501

In[43]:= Kappa[5 / 54]
Out[43]=
0.0631965

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In[44]:= Kappa[1 / 10]
Out[44]=
0.0682642

In[45]:= Kappa[1 / 100]
Out[45]=
0.00682382

In[46]:= Kappa[1 / 500]
Out[46]=
0.00136476

In[47]:= ListPlot[Table[{Th, Kappa[Th]}, {Th, 0, 1.5, 1 / 100}],
PlotRange -> {{0, 1.5}, {-0.4, 0.4}}]

In[48]:= ListPlot[Table[{Th, Kappa[Th] - (2 / 3) * Th}, {Th, 0, 0.8, 1 / 500}],

```

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