THE RIEMANN HYPOTHESIS AND THE TURÁN INEQUALITIES¹

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ABSTRACT. A solution is given to a fifty-eight year-old open problem of G. Pólya, involving the Taylor coefficients of the Riemann ξ -function.

1. Introduction. The purpose of this paper is to solve a fifty-eight year-old problem of Pólya [P, p. 16], related to the Riemann Hypothesis. This problem may be described as follows. Starting with Riemann's definition of his ξ -function (cf. Titchmarsh [T, p. 16], in a slightly different notation), i.e.,

(1.1)
$$\xi(iz) := \frac{1}{2} \left(z^2 - \frac{1}{4} \right) \pi^{-z/2 - 1/4} \Gamma\left(\frac{z}{2} + \frac{1}{4} \right) \xi\left(z + \frac{1}{2} \right),$$

where ζ is the Riemann zeta-function, then ξ is an entire function of order one and admits the integral representation (cf. [P, p. 11])

(1.2)
$$\xi\left(\frac{x}{2}\right) = 8\int_0^\infty \Phi(t)\cos(xt) dt,$$

where

(1.3)
$$\Phi(t) := \sum_{n=1}^{\infty} (2n^4\pi^2 e^{9t} - 3n^2\pi e^{5t}) \exp(-n^2\pi e^{4t}).$$

(We have dropped the usual factor of 4 in the definition of Φ .) From (1.2), the entire function ξ can be written in Taylor series form as

(1.4)
$$\frac{1}{8}\xi\left(\frac{x}{2}\right) = \sum_{m=0}^{\infty} \frac{(-1)^m \hat{b}_m x^{2m}}{(2m)!},$$

where

(1.5)
$$\hat{b}_m := \int_0^\infty t^{2m} \Phi(t) dt \qquad (m = 0, 1, ...).$$

On setting $z = -x^2$ in (1.4), the function F(z), defined by

(1.6)
$$F(z) := \sum_{m=0}^{\infty} \frac{\hat{b}_m z^m}{(2m)!},$$

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is an entire function of order $\frac{1}{2}$. If x_0 is a real zero of $\xi(x/2)$, then $z_0 := -x_0^2$ is a negative real zero of F(z) and the Riemann Hypothesis is equivalent to the statement that all the zeros of F(z) are real and negative. Now, it is known (cf. Boas [B, p. 24] or Pólya and Schur [PS]) that a necessary condition that F(z) have only real zeros is that

$$(1.7) \quad m \left(\frac{\hat{b}_m}{(2m)!}\right)^2 > (m+1) \frac{\hat{b}_{m-1}}{(2m-2)!} \frac{\hat{b}_{m+1}}{(2m+2)!} \qquad (m=1,2,\ldots),$$

or equivalently, that

(1.8)
$$(\hat{b}_m)^2 > \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} \qquad (m=1,2,\ldots).$$

(In today's terminology, the inequalities of (1.8) are commonly called *Turán inequalities*.)

In 1927, Pólya [P], while studying some fragmentary unpublished notes of J. L. W. V. Jensen dealing with the Riemann Hypothesis, raised the question of whether or not the Turán inequalities (1.8) are all valid. Our main result here is that these inequalities (1.8) are indeed all valid. Our interest in these inequalities (1.8) is very natural: if one of these inequalities (1.8) were to fail for some $m \ge 1$, then the Riemann Hypothesis could not be true!

The history concerning Pólya's problem of 1927 is very interesting. For nearly forty years, this problem was apparently untouched in the literature. Then, in 1966, Grosswald [G1, G2] generalized a formula of Hayman [Hay] on admissible functions, and, as an application of this generalization, Grosswald proved, in the notation of (1.8), that

$$(1.9) \quad (\hat{b}_m)^2 - \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} = \frac{(\hat{b}_m)^2}{m} \left\{1 + O\left(\frac{1}{\log m}\right)\right\} \quad \text{as } m \to \infty.$$

As the moments \hat{b}_m are necessarily positive (cf. (1.5) and (i) of Theorem A) for all $m \ge 1$, then Grosswald's result (1.9) proves that (1.8) is valid for all m sufficiently large, say $m \ge m_0$, but the value of m_0 was not determined from this analysis. To our knowledge, this gap in Grosswald's solution of Pólya's problem was subsequently not filled in the literature.

The delicate nature of the Turán inequalities (1.8) can be seen from the following calculation. As $\Phi(t)$ is positive for all $t \ge 0$ (cf. (i) of Theorem A), an application of the Cauchy-Schwarz inequality to (cf. (1.5))

$$\hat{b}_{m}^{2} = \left\{ \int_{0}^{\infty} t^{(2m-2)/2} \sqrt{\Phi(t)} \cdot t^{(2m+2)/2} \sqrt{\Phi(t)} dt \right\}^{2}$$

directly gives $(\hat{b}_m)^2 \leq \hat{b}_{m-1}\hat{b}_{m+1}$, which we equivalently write as

(1.10)
$$\hat{b}_m^2 \leqslant \left(\frac{2m+1}{2m+1}\right) \hat{b}_{m-1} \hat{b}_{m+1} \qquad (m=1,2,\ldots),$$

whereas the sought Turán inequalities (1.8) are nearly the reversed inequalities:

$$\hat{b}_m^2 > \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} \qquad (m=1,2,\ldots).$$

In [P], Pólya obtained some interesting results that relate the asymptotic behavior, as $t \to \infty$, of $\Phi(t)$ to the Riemann Hypothesis. In contrast, we focus our attention on the behavior of $\Phi(t)$ near t = 0, which requires, in our analysis, a detailed investigation of $\Phi(t)$, $\Phi'(t)$, $\Phi^{(2)}(t)$, and $\Phi^{(3)}(t)$ for t small. This analysis is carried out in §3. The various estimates developed in §3, while elementary in character, enable us to show in §3 that the function

(1.11)
$$K(t) := \int_{t}^{\infty} \Phi(\sqrt{u}) du \qquad (t \ge 0)$$

is such that $\log K(t)$ is strictly concave on $(0, +\infty)$. Having gathered these detailed calculations in §3, the basic ideas of the proof of our main result are given in §2. There, it is shown that if

(1.12)
$$\lambda_x := \frac{1}{\Gamma(x+1)} \int_0^\infty u^x K(u) du \qquad (x > -1),$$

then $\log \lambda_x$ is strictly concave on $(-1, +\infty)$, from which the validity of the Turán inequalities (1.8) for $m \ge 2$ are deduced. (The case m = 1 is settled numerically, the justifications for this being given in §4.)

In the subsequent sections, we repeatedly make use of several known properties of the function $\Phi(t)$, defined by (1.3). For the reader's convenience, we state the following theorem which summarizes some of the known properties of $\Phi(t)$.

THEOREM A. For the function $\Phi(t)$ of (1.3), write

$$\Phi(t) = \sum_{n=1}^{\infty} a_n(t),$$

where

$$(1.14) a_n(t) := \pi n^2 (2\pi n^2 e^{4t} - 3) \exp(5t - \pi n^2 e^{4t}) (n = 1, 2, ...).$$

Then, the following are valid:

- (i) for each $n \ge 1$, $a_n(t) > 0$ for all $t \ge 0$, so that $\Phi(t) > 0$ for all $t \ge 0$;
- (ii) $\Phi(z)$ is analytic in the strip $-\pi/8 < \text{Im } z < \pi/8$;
- (iii) $\Phi(t)$ is an even function, so that $\Phi^{(2m+1)}(0) = 0$ (m = 0, 1, ...);
- (iv) for any $\varepsilon > 0$,

$$\lim_{t\to\infty}\Phi^{(n)}(t)\exp[(\pi-\varepsilon)e^{4t}]=0$$

for each $n = 0, 1, \ldots$;

- (v) $\Phi'(t) < 0$ for all t > 0;
- (vi) $a'_n(t) < 0$ for all $t \ge 0$, for each n = 2, 3, ...;
- (vii) $a_1'(t) \ge 0$ for $0 \le t \le t_0$, and $a_1'(t) < 0$ for all $t > t_0$, where

(1.15)
$$t_0 := \frac{1}{4} \log \left[\frac{15 + \sqrt{105}}{8\pi} \right] = 0.001 \, 133 \, 489 \, 8 \, \cdots .$$

With the possible exception of (iii), the proofs of statements (i)-(iv) are elementary and can all be found in Pólya [P]. The proofs of statements (v)-(vii) can be found in Wintner [W].

The fact that $a'_1(t)$ changes sign (cf. (vii) of Theorem A) is important in our analysis, so we sketch the proofs of (vii) and (1.15). From (1.14),

(1.16)
$$a_1'(t) = -\pi \left[8\pi^2 e^{8t} - 30\pi e^{4t} + 15 \right] \exp(5t - \pi e^{4t}).$$

Now, the quantity in brackets above, a quadratic polynomial in e^{4t} , has precisely one positive zero t_0 , which is given in (1.15). It then follows that $a_1'(t) \ge 0$ for $0 \le t \le t_0$, and that $a_1'(t) < 0$ for $t > t_0$, which is the desired conclusion (vii) of Theorem A.

2. Basic results. Our basic result, Theorem 2.5, gives that the Turán inequalities (1.8) are all valid, thereby completely solving Pólya's problem. The proof of this result depends in part on a large number of easy but lengthy mathematical calculations (not numerical computations) which might detract from the basic ideas of the proof. These results (Lemmas 3.1-3.12) have been gathered separately in §3. In this section, we give the essential ideas leading to the proof of Theorem 2.5.

We begin with Proposition 2.1, which makes use of Lemma 3.12, to be established in §3.

PROPOSITION 2.1. With $\Phi(t)$ defined in (1.3), set

(2.1)
$$K(t) := \int_{t}^{\infty} \Phi(\sqrt{u}) du \qquad (t \ge 0).$$

Then, $\log K(t)$ is strictly concave on $(0, +\infty)$, i.e.,

(2.2)
$$\frac{d^2 \log K(t)}{dt^2} < 0 \qquad (t > 0).$$

PROOF. With (2.1), it can be verified that

$$\frac{d^2 \log K(t)}{dt^2} = -\frac{\left(\int_t^{\infty} \Phi(\sqrt{u}) du\right) \Phi'(\sqrt{t}) / 2\sqrt{t} + \left(\Phi(\sqrt{t})\right)^2}{\left(\int_t^{\infty} \Phi(\sqrt{u}) du\right)^2} \qquad (t > 0).$$

As the denominator of the fraction above is positive for all t > 0 (cf. (i) of Theorem A), then (2.2) holds iff

$$(2.3) V(t) := \left(\int_t^\infty \Phi(\sqrt{u}) du \right) \frac{\Phi'(\sqrt{t})}{2\sqrt{t}} + \left(\Phi(\sqrt{t}) \right)^2 > 0 (t > 0),$$

or equivalently, iff

(2.4)
$$tV(t^2) = \left(\int_{t}^{\infty} s\Phi(s) \, ds\right) \Phi'(t) + t(\Phi(t))^2 > 0 \qquad (t > 0).$$

But, on setting

(2.5)
$$J(t) := \int_{t}^{\infty} s\Phi(s) ds \qquad (t \ge 0),$$

and

(2.6)
$$g(t) := J(t)\Phi'(t) + t(\Phi(t))^2 \qquad (t \ge 0),$$

then (2.4) simply becomes

$$(2.7) g(t) > 0 (t > 0),$$

which is the conclusion of Lemma 3.12 of §3. \Box

We remark that the results established in §3 similarly allow us to deduce that if

$$(2.8) I(t) := \int_{t}^{\infty} \Phi(s) ds (t \ge 0),$$

then $\log I(t)$ is also strictly concave on $(0, +\infty)$. This result is, however, not strong enough for our purposes to deduce the Turán inequalities of (1.8).

A specific elementary property of strictly concave functions, needed in the subsequent proof, is given in

LEMMA 2.2. Let I be an open (bounded or unbounded) interval, and let $h(x) \in C^2(I)$ be strictly concave on I (i.e., $h^{(2)}(x) < 0$ for $x \in I$). Then, for any four points a, b, c, d in I with a < c < d < b,

$$\frac{h(c)-h(a)}{c-a} > \frac{h(b)-h(d)}{b-d}.$$

If, in addition, c - a = b - d, then

$$(2.10) h(c) + h(d) > h(a) + h(b).$$

PROOF. Let a, b, c, d be any four points of I with a < c < d < b, and with corresponding points P, Q, R, S on the graph of h, as shown in Figure 1. Since $h^{(2)}(x) < 0$, it follows that

$$slope(PQ) > slope(PR) > slope(QR) > slope(RS),$$

whence slope(PQ) > slope(RS), which gives (2.9). If c - a = b - d, then (2.10) follows immediately from (2.9). \Box

A special case (m = 2) of a problem of Pólya and Szegö [PSz, Part II, Problem 68] is the following lemma. (A more general version of this result appears in Karlin [K, p. 17].)

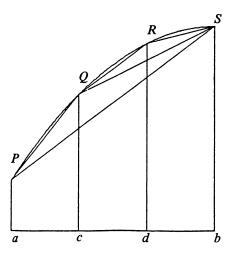


FIGURE 1

LEMMA 2.3. Let $f_1(t)$, $f_2(t)$, $\phi_1(t)$ and $\phi_2(t)$ be continuous and absolutely integrable on $[0, +\infty)$. Suppose further that $f_i(t)\phi_j(t)$ $(1 \le i, j \le 2)$ and $f_1(t)f_2(t)\phi_1(t)\phi_2(t)$ are absolutely integrable on $[0, +\infty)$. Then,

(2.11)
$$\det \begin{bmatrix} \int_{0}^{\infty} f_{1}(t) \phi_{1}(t) dt & \int_{0}^{\infty} f_{1}(t) \phi_{2}(t) dt \\ \int_{0}^{\infty} f_{2}(t) \phi_{1}(t) dt & \int_{0}^{\infty} f_{2}(t) \phi_{2}(t) dt \end{bmatrix} \\ = \iint_{0 < u < v < +\infty} \det \begin{bmatrix} f_{1}(u) & f_{1}(v) \\ f_{2}(u) & f_{2}(v) \end{bmatrix} \cdot \det \begin{bmatrix} \phi_{1}(u) & \phi_{1}(v) \\ \phi_{2}(u) & \phi_{2}(v) \end{bmatrix} du dv.$$

In the proof of the next result, it will be convenient to adopt the following notation. Let X and Y be subsets of \mathbb{R} , and let f be a real-valued function on $X \times Y$. Then, for $x_1, x_2 \in X$ with $x_1 < x_2$, and for $y_1, y_2 \in Y$ with $y_1 < y_2$, set

(2.12)
$$f\begin{pmatrix} x_1 & x_2 \\ y_1 & y_2 \end{pmatrix} := \det \begin{bmatrix} f(x_1, y_1) & f(x_1, y_2) \\ f(x_2, y_1) & f(x_2, y_2) \end{bmatrix}.$$

PROPOSITION 2.4. With K(t) defined in (2.1), set

(2.13)
$$\lambda_x := \frac{1}{\Gamma(x+1)} \int_0^\infty u^x K(u) du \qquad (x > -1),$$

where $\Gamma(t)$ denotes the gamma function. Then, $\log \lambda_x$ is strictly concave on $(-1, +\infty)$.

PROOF. For any real numbers $s, t > -\frac{1}{2}$, the classical formula connecting the beta function with the gamma function gives the identity

$$\frac{u^{s+t}}{\Gamma(s+t+1)} = \int_0^u \frac{v^{s-1/2}}{\Gamma(s+1/2)} \cdot \frac{(u-v)^{t-1/2}}{\Gamma(t+1/2)} dv.$$

Substituting the above identity in (2.13), with x replaced by s + t and with y := u - v, gives

$$\lambda_{s+t} = \int_0^\infty \frac{v^{s-1/2}}{\Gamma(s+1/2)} \int_0^\infty \frac{y^{t-1/2}}{\Gamma(t+1/2)} K(v+y) \, dy \, dv,$$

which we write as

(2.14)
$$\lambda_{s+t} = \int_0^\infty \frac{x^{s-1/2}}{\Gamma(s+1/2)} L_t(x) dx,$$

where

(2.15)
$$L_{t}(x) := \int_{0}^{\infty} \frac{y^{t-1/2}}{\Gamma(t+1/2)} K(x+y) \, dy.$$

We also set

(2.16)
$$\Theta_{x}(y) := K(x+y); \qquad G_{t}(y) := \frac{y^{t-1/2}}{\Gamma(t+1/2)},$$

where x, y > 0 and $t > -\frac{1}{2}$. With the notation of (2.12), we next note that Lemma 2.3, applied to the integral of (2.15), can be expressed as

$$(2.17) L\begin{pmatrix} x_1 & x_2 \\ t_1 & t_2 \end{pmatrix} = \iint_{0 \le u \le v \le \infty} \Theta\begin{pmatrix} x_1 & x_2 \\ u & v \end{pmatrix} G\begin{pmatrix} t_1 & t_2 \\ u & v \end{pmatrix} du dv.$$

Now, a direct computation shows that if 0 < u < v and if $t_1 < t_2$ (where $t_i > -\frac{1}{2}$), then

$$(2.18) G\begin{pmatrix} t_1 & t_2 \\ u & v \end{pmatrix} = \frac{u^{t_1 - 1/2} v^{t_1 - 1/2}}{\Gamma(t_1 + 1/2) \Gamma(t_2 + 1/2)} \left[v^{t_2 - t_1} - u^{t_2 - t_1} \right] > 0.$$

We next show that

(2.19)
$$L\begin{pmatrix} x_1 & x_2 \\ t_1 & t_2 \end{pmatrix} < 0 \qquad (0 < x_1 < x_2; -\frac{1}{2} < t_1 < t_2).$$

To establish (2.19), we see from (2.17) and (2.18) that it suffices to establish that

(2.20)
$$\Theta\begin{pmatrix} x_1 & x_2 \\ u & v \end{pmatrix} < 0 \qquad (0 < x_1 < x_2; 0 < u < v).$$

For any x_1 , x_2 , u, v satisfying $0 < x_1 < x_2$ and 0 < u < v, set

(2.21)
$$a := x_1 + u$$
, $b := x_2 + v$, $c := x_2 + u$ and $d := x_1 + v$,

so that

$$a < c < b$$
, $a < d < b$ and $c - a = b - d$.

Since $\log K(t)$ is strictly concave on $(0, +\infty)$ from Proposition 2.1, we deduce from Lemma 2.2 that (cf. (2.10))

$$\log K(c) + \log K(d) > \log K(a) + \log K(b),$$

or

Thus, with the definitions of (2.21), this becomes

(2.22)
$$K(x_2 + u)K(x_1 + v) > K(x_1 + u)K(x_2 + v).$$

On the other hand, from (2.12), (2.16) and (2.22), we have

$$\Theta\begin{pmatrix} x_1 & x_2 \\ u & v \end{pmatrix} = \det \begin{bmatrix} \Theta_{x_1}(u) & \Theta_{x_1}(v) \\ \Theta_{x_2}(u) & \Theta_{x_2}(v) \end{bmatrix}
= K(x_1 + u)K(x_2 + v) - K(x_1 + v)K(x_2 + u) < 0,$$

which establishes (2.20).

Next, using (2.13), set $\Lambda(s,t) := \lambda_{s+t}$ (where $s > -\frac{1}{2}, t > -\frac{1}{2}$). Again from Lemma 2.3, for any $-\frac{1}{2} < t_1 < t_2$ and $\frac{1}{2} < s_1 < s_2$, the notation (2.12) permits us to write (2.14) in the form

(2.23)
$$\Lambda \begin{pmatrix} s_1 & s_2 \\ t_1 & t_2 \end{pmatrix} = \iint_{0 \le u \le v \le \infty} G \begin{pmatrix} s_1 & s_2 \\ u & v \end{pmatrix} L \begin{pmatrix} t_1 & t_2 \\ u & v \end{pmatrix} du dv.$$

Now, from (2.18),

$$G\begin{pmatrix} s_1 & s_2 \\ u & v \end{pmatrix} > 0,$$

and from (2.19),

$$L\begin{pmatrix} t_1 & t_2 \\ u & v \end{pmatrix} < 0.$$

Thus, it follows from (2.23) that

$$\Lambda \begin{pmatrix} s_1 & s_2 \\ t_1 & t_2 \end{pmatrix} < 0 \qquad \left(-\frac{1}{2} < s_1 < s_2; -\frac{1}{2} < t_1 < t_2 \right),$$

or equivalently, that

(2.24)
$$\lambda_{s_1+t_1}\lambda_{s_2+t_2} - \lambda_{s_1+t_2}\lambda_{s_2+t_1} < 0.$$

On setting $s_1 = t_1 = u/2$ and $s_2 = t_2 = v/2$ (where -1 < u < v), inequality (2.24) becomes

$$\lambda_{(u+v)/2}^2 > \lambda_u \lambda_v,$$

which implies that $\log \lambda_x$ is strictly concave on $(-1, +\infty)$. \square

This brings us to our main result:

THEOREM 2.5. The Turán inequalities (1.8), i.e.,

(2.26)
$$(\hat{b}_m)^2 > \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} (m=1,2,...),$$

are all valid (where \hat{b}_m is defined in (1.5)).

PROOF. The strict concavity of $\log \lambda_x$ on $(-1, +\infty)$, from Proposition 2.4, gives that

(2.27)
$$\lambda_{m-1/2}^2 > \lambda_{m-3/2} \lambda_{m+1/2} \qquad (m = 1, 2, ...).$$

Now, since an integration by parts and the change of variables $u = t^2$ in (2.13) yield

(2.28)
$$\lambda_x = \frac{2}{\Gamma(x+2)} \int_0^\infty t^{2x+3} \Phi(t) dt,$$

(2.27) becomes, from the definition of \hat{b}_m in (1.5), just

(2.29)
$$(\hat{b}_{m+1})^2 > \left(\frac{2m+1}{2m+3}\right) \hat{b}_m \hat{b}_{m+2} \qquad (m=1,2,\ldots),$$

or equivalently,

(2.30)
$$(\hat{b}_m)^2 > \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} (m=2,3,...).$$

Thus, (2.30) establishes the desired result of (2.26), except for the case m = 1. This remaining case, m = 1, of the Turán inequalities (1.8) is then settled numerically, as follows. The numbers $\{\hat{b}_m\}_{m=0}^2$ were determined by Romberg integration to an accuracy exceeding fifty decimal places, and the associated Turán difference, namely,

(2.31)
$$(\hat{b}_1)^2 - \frac{1}{3}\hat{b}_0\hat{b}_2 = 3.5884 \cdots 10^{-8} > 0,$$

was determined. (The details giving rigorous error bounds for these numerical calculations appear in $\S4$.) Thus, (2.30) and (2.31) give the desired result of (2.26). \Box

We have in fact numerically determined the moments $\{\hat{b}_m\}_{m=0}^{20}$, each to an accuracy of fifty decimal places, as well as the associated *Turán differences*, $\{D_m\}_{m=1}^{19}$,

where

(2.32)
$$D_m := (\hat{b}_m)^2 - \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1}.$$

These numbers have been included in §4 for the benefit of the reader.

3. Background analysis. The purpose of this section is to obtain precise estimates for the functions $\Phi(t)$, $\Phi'(t)$, $\Phi^{(2)}(t)$ and $\Phi^{(3)}(t)$, where $\Phi(t)$ is defined in (1.13) and (1.14). For convenience, we will adhere to the following notations. For $t \ge 0$, set

(3.1)
$$a_n(t) := \pi n^2 (2\pi n^2 e^{4t} - 3) \exp(5t - \pi n^2 e^{4t})$$
 $(n = 1, 2, ...),$

$$\Phi(t) := \sum_{n=1}^{\infty} a_n(t)$$

and

$$\Phi_1(t) := \sum_{n=2}^{\infty} a_n(t).$$

LEMMA 3.1. Setting

(3.4)
$$I(t) := \int_{t}^{\infty} \Phi(y) \, dy \qquad (t \ge 0),$$

then

$$(3.5) I(t) = \frac{\pi}{2} \exp(5t - \pi e^{4t}) - \frac{1}{8\pi^{1/4}} \int_{\pi e^{4t}}^{\infty} y^{1/4} e^{-y} dy + \int_{t}^{\infty} \Phi_{1}(y) dy.$$

PROOF. From (3.2)–(3.4), $I(t) = \int_t^\infty a_1(y) dy + \int_t^\infty \Phi_1(y) dy$. From (3.1), the integral $\int_t^\infty a_1(y) dy$ consists of the difference of two terms. Integrating each of these by parts and adding the results yields the desired result of (3.5). \square

In the next result, upper and lower estimates for I(t) of (3.4) are derived.

LEMMA 3.2. With the definition of (3.4),

$$(3.6) I(t) > \frac{\pi}{2} \exp(5t - \pi e^{4t}) \left[1 - \frac{1}{4\pi} e^{-4t} - \frac{1}{16\pi^2} e^{-8t} \right] (t \ge 0)$$

and

(3.7)
$$I(t) < \frac{\pi}{2} \exp(5t - \pi e^{4t}) \qquad (t \ge 0).$$

PROOF. From Theorem A(i), it follows that $\Phi_1(t) > 0$ for all $t \ge 0$. Thus, $\int_t^{\infty} \Phi_1(s) ds > 0$ for all $t \ge 0$. Thus, from (3.5) of Lemma 3.1,

$$I(t) > \frac{\pi}{2} \exp(5t - \pi e^{4t}) - \frac{1}{8\pi^{1/4}} \int_{\pi e^{4t}}^{\infty} y^{1/4} e^{-y} dy \qquad (t \ge 0).$$

Applying integration by parts to the last integral above yields

(3.8)
$$I(t) > \frac{\pi}{2} \exp(5t - \pi e^{4t}) - \frac{1}{8} \exp(t - \pi e^{4t}) - \frac{1}{32\pi^{1/4}} \int_{\pi e^{4t}}^{\infty} y^{-3/4} e^{-y} dy.$$

Next, for the complementary incomplete gamma function

$$\Gamma(\nu; x) := \int_{x}^{\infty} y^{\nu-1} e^{-y} dy \qquad (0 < x < \infty, \nu < 1),$$

it is known (cf. Luke [L, p. 201]) that

$$\Gamma(\nu; x) \le \left(\frac{x+1}{x+2-\nu}\right) x^{\nu-1} e^{-x} \qquad (0 < x < \infty, \nu < 1).$$

Choosing $\nu = \frac{1}{4}$ and $x = \pi e^{4t}$ and applying this inequality to the last integral of (3.8) then directly gives the desired lower bound (3.6) of Lemma 3.2.

Next, Haviland [Hav, p. 415] proved that $\Phi_1(t)$ of (3.3) satisfies

(3.9)
$$\Phi_1(s) < 64\pi^2 \exp(9s - 4\pi e^{4s}) \qquad (s \ge 0).$$

Inserting the above inequality into the last integral of (3.5) then yields

(3.10)
$$I(t) < \frac{\pi}{2} \exp(5t - \pi e^{4t}) - \frac{1}{8\pi^{1/4}} \int_{\pi e^{4t}}^{\infty} y^{1/4} e^{-y} dy + \frac{16}{\pi^{1/4}} \int_{\pi e^{4t}}^{\infty} y^{5/4} e^{-4y} dy.$$

Next, since ye^{-3y} is strictly decreasing for $y > \frac{1}{3}$, one obtains the elementary inequality

$$v^{5/4}e^{-4y} < \pi e^{-3\pi}v^{1/4}e^{-y} \qquad (y > \pi).$$

Applying the above inequality to the integrand of the last integral in (3.10), (3.10) then becomes

$$(3.11) I(t) < \frac{\pi}{2} \exp(5t - \pi e^{4t}) + \left(-\frac{1}{8\pi^{1/4}} + \frac{16\pi^{3/4}}{e^{3\pi}}\right) \int_{\pi e^{4t}}^{\infty} y^{1/4} e^{-y} dy.$$

But as $16\pi^{3/4}/e^{3\pi} < 1/8\pi^{1/4}$, i.e., $128\pi e^{-3\pi} (=0.032451\cdots) < 1$, the last term in (3.11) is negative, whence $I(t) < (\pi/2) \exp(5t - \pi e^{4t})$ for all $t \ge 0$, the desired inequality of (3.7). \square

LEMMA 3.3. With the definition of (3.3),

$$|\Phi_1'(t)| < 565\pi^3 \exp(13t - 4\pi e^{4t}) \qquad (t \ge 0).$$

PROOF. From (3.1) and (3.3),

$$\left|\Phi_1'(t)\right| = \left|\sum_{n=2}^{\infty} \pi n^2 (8\pi^2 n^4 e^{8t} - 30\pi n^2 e^{4t} + 15) \exp(5t - \pi n^2 e^{4t})\right| \qquad (t \ge 0),$$

or equivalently, with x := e', (3.13)

$$\left|\Phi_1'(t)\right| = 8\pi^3 x^5 \left| \sum_{n=2}^{\infty} n^6 \left(x^8 - \frac{15}{4\pi n^2} x^4 + \frac{15}{8\pi^2 n^4} \right) \exp(-\pi n^2 x^4) \right| \qquad (x \ge 1).$$

It is easily verified that $-15x^4/4\pi n^2 + 15/8\pi^2 n^4 < 0$ for all $x \ge 1$ and all $n \ge 2$, so that, with $y := \pi x^4$, (3.13) becomes

(3.14)
$$\left|\Phi_1'(t)\right| < \frac{8y^{13/4}}{\pi^{1/4}} \sum_{n=2}^{\infty} n^6 e^{-n^2 y} \qquad (y \ge \pi).$$

As $n^6 e^{-n^2 y}$ is a monotone decreasing function of $n \ge 2$ for each fixed value of $y \ge \pi$, then by the integral test, we have that

$$\sum_{n=2}^{\infty} n^6 e^{-n^2 y} < 64 e^{-4 y} + \int_2^{\infty} s^6 e^{-s^2 y} ds.$$

On making the substitution $u := s^2y$ in the above integral and on integrating by parts three times, we obtain

$$\sum_{n=2}^{\infty} n^6 e^{-n^2 y} < 64 e^{-4y} + \frac{e^{-4y}}{2y^{7/2}} \left\{ (4y)^{5/2} + \frac{5}{2} (4y)^{3/2} + \frac{15}{4} (4y)^{1/2} + \frac{15e^{4y}}{8} \int_{4y}^{\infty} \frac{e^{-u}}{\sqrt{u}} du \right\}.$$

Since $1/\sqrt{u} < 1$ for all $u \ge 4y \ge 4\pi$, then $e^{4y} \int_{4y}^{\infty} e^{-u} du / \sqrt{u} < 1$, so that the above inequality becomes

$$\sum_{n=2}^{\infty} n^6 e^{-n^2 y} < 64 e^{-4y} \left\{ 1 + \frac{1}{4y} + \frac{5}{32y^2} + \frac{15}{256y^3} + \frac{15}{1024y^{7/2}} \right\} \qquad (y \ge \pi).$$

Now, the quantity in braces above is monotone decreasing for $y \ge \pi$, and the value of this quantity when $y = \pi$ is bounded above by $1 + (13/40\pi)$. Thus, we have

$$\sum_{n=2}^{\infty} n^6 e^{-n^2 y} < 64 e^{-4 y} \left\{ 1 + \frac{13}{40 \pi} \right\} \qquad (y \ge \pi),$$

so that, from (3.14) and the fact that $y = \pi e^{4t}$.

$$\left| \Phi_1'(t) \right| < 512 \left(1 + \frac{13}{40\pi} \right) \pi^3 \exp(13t - 4\pi e^{4t})$$

$$< 565\pi^3 \exp(13t - 4\pi e^{4t}) \qquad (t \ge 0),$$

the desired inequality of (3.12). \Box

LEMMA 3.4. With the definition of (3.3),

$$(3.15) \quad \int_{t}^{\infty} ds \int_{s}^{\infty} \Phi_{1}(y) \, dy < \frac{1}{32\pi^{1/4}} \int_{t}^{\infty} ds \int_{\pi e^{4s}}^{\infty} y^{-3/4} e^{-y} \, dy \qquad (t \ge 0).$$

PROOF. By Haviland's upper estimate (3.9) for $\Phi_1(s)$ and the substitution $v := \pi e^{4y}$,

(3.16)
$$\int_{t}^{\infty} ds \int_{s}^{\infty} \Phi_{1}(y) dy < \frac{16}{\pi^{1/4}} \int_{t}^{\infty} ds \int_{\pi^{0/4}}^{\infty} v^{5/4} e^{-4v} dv \qquad (t \ge 0).$$

Next, since v^2e^{-3v} is strictly decreasing for $v \ge \pi$, one obtains the elementary inequalities

$$v^{5/4}e^{-4v} \leqslant \frac{\pi^2 v^{-3/4}e^{-v}}{e^{3\pi}} < \frac{v^{-3/4}e^{-v}}{512} \qquad (v \geqslant \pi),$$

which, when applied to (3.16), directly gives the desired result of (3.15). \Box

LEMMA 3.5. With the definition of (3.2), set

(3.17)
$$J(t) := \int_{t}^{\infty} s\Phi(s) ds \qquad (t \ge 0).$$

Then,

(3.18)
$$J(t) < \left\{ \frac{\pi t}{2} + \frac{e^{-4t}}{8} \right\} \exp(5t - \pi e^{4t}) \qquad (t \ge 0).$$

PROOF. An integration by parts shows, with (3.4), that

(3.19)
$$J(t) = tI(t) + \int_t^{\infty} I(s) ds.$$

Now, with the expression (3.5) of Lemma 3.1, with one integration by parts, and with some easy simplifications,

$$\int_{t}^{\infty} I(s) ds = \frac{1}{8} \exp(t - \pi e^{4t}) - \frac{1}{32\pi^{1/4}} \int_{t}^{\infty} ds \int_{\pi e^{4s}}^{\infty} y^{-3/4} e^{-y} dy + \int_{t}^{\infty} ds \int_{s}^{\infty} \Phi_{1}(y) dy.$$

Thus, on applying inequality (3.15) of Lemma 3.4 to the above expression, we obtain

(3.20)
$$\int_{t}^{\infty} I(s) ds < \frac{1}{8} \exp(t - \pi e^{4t}) \qquad (t \ge 0).$$

Then, applying (3.20) and the upper bound (3.7) of Lemma 3.2 to (3.19) directly gives the desired inequality of (3.18). \Box

Our proof in Proposition 2.1 of the strict concavity of $\log K(t)$ on $(0, +\infty)$, where (cf. (2.1))

$$K(t) := \int_{t}^{\infty} \Phi(\sqrt{u}) du \qquad (t \ge 0),$$

is based on the assertion that the function g(t), defined (cf. (3.26)) by

$$g(t) := J(t)\Phi'(t) + t[\Phi(t)]^2 \qquad (t \geqslant 0),$$

is positive for all t > 0. The proof of this assertion will be divided into the two cases:

$$(3.21) g(t) > 0 for t \in (0, 0.01]$$

and

$$(3.22) g(t) > 0 for t > 0.01.$$

The case of (3.22) will be a consequence of previously established estimates. For the case of (3.21), we first note that since $\Phi'(0) = 0$ (cf. (iii) of Theorem A), g(0) = 0 by (3.26). By Taylor's formula, we can then write

(3.23)
$$g(t) = t \left[g'(0) + \frac{g^{(2)}(\xi)t}{2} \right] \qquad (\xi \in (0, t); 0 < t \le 0.01).$$

Consequently, in order to establish (3.21), it suffices to show that

(3.24)
$$g'(0) + \frac{g^{(2)}(\xi)t}{2} > 0 \qquad (\xi \in (0, t); 0 < t \le 0.01).$$

This last inequality requires that we estimate g'(0) and $g^{(2)}(t)$ for $0 < t \le 0.01$. Since by (3.26),

(3.25)
$$g^{(2)}(t) = 3\Phi'(t)\Phi(t) + t[\Phi'(t)]^2 + J(t)\Phi^{(3)}(t),$$

it is also necessary to examine the behavior of $\Phi^{(3)}(t)$ on [0,0.01]. We remark that the *main reason* for concentrating on this particular interval [0,0.01] is that it is relatively easy to prove that $\Phi^{(3)}(t) \ge 0$ on this interval.

Preliminaries aside, we proceed to establish some lemmas for establishing (3.21). The reader may find it useful to have a hand calculator available while reading portions of what follows.

LEMMA 3.6. With the definitions of (3.2) and (3.17), set

(3.26)
$$g(t) := J(t)\Phi'(t) + t[\Phi(t)]^2 \qquad (t \ge 0).$$

Then,

$$\Phi(0) > 0.446696899\cdots,$$

$$\Phi^{(2)}(0) > -33.461010\cdots,$$

and

$$(3.29) g'(0) > 0.018790450 \cdots$$

PROOF. From (3.2) and (i) of Theorem A, it follows that $\Phi(0) > a_1(0) + a_2(0)$. Simply evaluating $a_1(0)$ and $a_2(0)$ and adding, yields the result of (3.27). Next, from (3.2), we have $\Phi^{(2)}(t) = \sum_{n=1}^{\infty} a_n^{(2)}(t)$, where from (3.1),

(3.30)
$$a_n^{(2)}(0) = \pi n^2 [32\pi^3 n^6 - 224\pi^2 n^4 + 330\pi n^2 - 75] \exp(-\pi n^2).$$

With $x := \pi n^2$, the quantity in brackets above is a cubic polynomial in x, having three distinct zeros $0.277455812\cdots$, $1.672823383\cdots$, and $5.049720804\cdots$. Since $x = \pi n^2 > 5.049720804\cdots$ for all $n \ge 2$, then $a_n^{(2)}(0) > 0$ for all $n \ge 2$. Thus, a lower estimate for $\Phi^{(2)}(0)$ is given by

$$\Phi^{(2)}(0) > a_1^{(2)}(0) + a_2^{(2)}(0).$$

Evaluating $a_1^{(2)}(0)$ and $a_2^{(2)}(0)$ from (3.30) and adding then yields the result of (3.28). To derive (3.29), the definition of g(t) in (3.26) provides us with

(3.31)
$$g'(t) = t\Phi'(t)\Phi(t) + J(t)\Phi^{(2)}(t) + [\Phi(t)]^2 \qquad (t \ge 0),$$

so that

(3.32)
$$g'(0) = J(0)\Phi^{(2)}(0) + [\Phi(0)]^2.$$

Now, $J(0) < e^{-\pi}/8 = 0.0005401739 \cdots$ from (3.18) of Lemma 3.5, and applying this inequality (along with those established in (3.27)–(3.28)) in (3.32) yields the last inequality, (3.29), of Lemma 3.6. \Box

LEMMA 3.7. With the definition of (3.2),

(3.33)
$$\Phi^{(3)}(t) > 0 \qquad (0 < t \le 0.01).$$

PROOF. Since $\Phi^{(3)}(0) = 0$ from (iii) of Theorem A, it suffices to show that $\Phi^{(4)}(t) > 0$ on [0, 0.01]. From (3.2), it follows that

(3.34)
$$\Phi^{(4)}(t) = \sum_{n=1}^{\infty} a_n^{(4)}(t) = \sum_{n=1}^{\infty} \pi n^2 \exp(5t - \pi n^2 e^{4t}) p_5(\pi n^2 e^{4t}),$$

where

$$(3.35) \quad p_5(x) := 512x^5 - 8,448x^4 + 41,408x^3 - 68,096x^2 + 30,930x - 1,875.$$

The above polynomial has five distinct zeros, given by $0.071\ 349 \cdots$, $0.604\ 398 \cdots$, $1.996\ 885 \cdots$, $4.617\ 597 \cdots$, and $9.209\ 769 \cdots$, so that $p_5(x) > 0$ for x > 9.210. As $\pi n^2 > 9.210$ for all $n \ge 2$, it follows from (3.34) that

$$a_n^{(4)}(t) > 0$$
 $(n \ge 2, t \ge 0),$

so that

(3.36)
$$\Phi^{(4)}(t) > a_1^{(4)}(t) \qquad (t \ge 0).$$

Thus, it suffices to show that $a_1^{(4)}(t) = \pi \exp(5t - \pi e^{4t}) \cdot p_5(\pi e^{4t})$ is positive on [0, 0.01].

The derivative of the polynomial $p_5(x)$ (cf. (3.35)) has four distinct zeros, given by $0.30515\cdots$, $1.3791\cdots$, $3.6496\cdots$, and $7.8660\cdots$. In particular, $p_5(x)$ is thus increasing on the interval $(1.3791\cdots, 3.6496\cdots)$. Since πe^{4t} falls in this latter interval for all $0 \le t \le 0.01$, then $p_5(\pi e^{4t}) \ge p_5(\pi)$ for all $0 \le t \le 0.01$. Similarly, since $\exp(5t - \pi e^{4t})$ is decreasing for all $t \ge 0$, we then have

$$(3.37) a_1^{(4)}(t) > \pi \exp(.05 - \pi e^{.04}) \cdot p_5(\pi) > 5{,}133 (0 \le t \le 0.01).$$

Consequently (cf. (3.36)), $\Phi^{(4)}(t) > 0$ for all $0 \le t \le 0.01$, which gives the desired inequality (3.33). \square

Since our goal is to estimate $g^{(2)}(t)$ on the interval [0, 0.01], and since the expression for $g^{(2)}(t)$ involves the term $3\Phi'(t)\Phi(t)$ (cf. (3.25)), we next derive an estimate for $3\Phi'(t)\Phi(t)$.

LEMMA 3.8. We have

$$|3\Phi'(t)\Phi(t)| \le 0.506 \qquad (0 \le t \le 0.01).$$

PROOF. By definition (cf. (3.2) and (3.3)),

(3.39)
$$\Phi(t) = a_1(t) + \Phi_1(t) \qquad (t \ge 0),$$

and we first show that

(3.40)
$$\Phi_1(t) < \frac{1}{202} a_1(t) \qquad (t \ge 0).$$

Since $\Phi_1(t) < 64\pi^2 \exp(9t - 4\pi e^{4t})$ for all $t \ge 0$ from (3.9), to establish (3.40) it suffices to show that

$$64\pi^2 \exp(9t - 4\pi e^{4t}) < \frac{1}{202}a_1(t) \qquad (t \ge 0),$$

or equivalently (cf. (3.1)),

$$6464 \exp(-3\pi e^{4t}) < 1 - \frac{3}{2\pi e^{4t}} \qquad (t \ge 0).$$

As is easily seen, the above inequality is valid for all $t \ge 0$ if it holds for t = 0:

$$(.521\,641\,681\,\cdots\,=)6464e^{-3\pi}<1\,-\,\frac{3}{2\pi}(=\,.522\,535\,170\,\cdots).$$

As this is valid (3.40) then follows. Consequently, combining (3.39) and (3.40) gives (with (i) of Theorem A),

(3.41)
$$0 < \Phi(t) < \frac{203}{202} a_1(t) \qquad (t \ge 0).$$

Continuing, from (3.1), we see that

$$a_1(t) = 2\pi^2 \left(1 - \frac{3}{2\pi e^{4t}}\right) \exp(9t - \pi e^{4t}) \le 2\pi^2 \left(1 - \frac{3}{2\pi e^{.04}}\right) \exp(9t - \pi e^{4t})$$

for $0 \le t \le 0.01$, so that

$$a_1(t) \le 1.082513669\pi^2 \exp(9t - \pi e^{4t})$$
 $(0 \le t \le 0.01)$.

Thus, from (3.41), there follows

$$(3.42) 0 < \Phi(t) < 1.087872648\pi^2 \exp(9t - \pi e^{4t}) (0 \le t \le 0.01).$$

We next estimate $\Phi'(t) = a_1'(t) + \Phi_1'(t)$. Recalling from (vii) of Theorem A that $a_1'(t) \ge 0$ for $0 \le t \le t_0$, where t_0 is explicitly given in (1.15), then, as $\Phi'(t) < 0$ for all t > 0 (cf. (v) of Theorem A), we have

$$0 \geqslant \Phi'(t) = a_1'(t) + \Phi_1'(t) \geqslant \Phi_1'(t) = -|\Phi_1'(t)| \qquad (0 \leqslant t \leqslant t_0),$$

so that

$$|\Phi'(t)| \leq |\Phi'_1(t)| \qquad (0 \leq t \leq t_0).$$

Hence, from (3.42), (3.43) and the upper bound (3.12) for $|\Phi'_1(t)|$, we have

$$3|\Phi'(t)\Phi(t)| \le 3(1.087872648\pi^2 \exp(9t - \pi e^{4t}))565\pi^3 \exp(13t - 4\pi e^{4t})$$

for $0 \le t \le t_0$, i.e.,

$$3|\Phi'(t)\Phi(t)| \le 1,843.944138\pi^{5}\exp(22t - 5\pi e^{4t}) \qquad (0 \le t \le t_0).$$

As $\exp(22t - 5\pi e^{4t})$ is strictly decreasing for all $t \ge 0$, then

$$3|\Phi'(t)\Phi(t)| \le 1.843.944138\pi^5 e^{-5\pi} \le 0.085038454$$
 $(0 \le t \le t_0)$

so that certainly

(3.44)
$$3|\Phi'(t)\Phi(t)| \le 0.506 \quad (0 \le t \le t_0).$$

On the other hand, if $t_0 \le t \le 0.01$, from (3.42), (3.2) and (3.3),

$$(3.45) \quad 3|\Phi'(t)\Phi(t)| \leq 3(1.087872648\pi^2 \exp(9t - \pi e^{4t})) (|a_1'(t)| + |\Phi_1'(t)|).$$

At this point, we need an upper bound for $|a_1'(t)|$. Clearly, from (3.1),

$$|a_1'(t)| = \pi |8\pi^2 e^{8t} - 30\pi e^{4t} + 15|\exp(5t - \pi e^{4t})|$$

$$= 8\pi^3 \left(1 - \frac{15}{4\pi e^{4t}} + \frac{15}{8\pi^2 e^{8t}}\right) \exp(13t - \pi e^{4t}).$$

Next, if we set

$$\Theta(t) := 1 - \frac{15}{4\pi e^{4t}} + \frac{15}{8\pi^2 e^{8t}},$$

it is easily seen that

$$\max_{0 \le t \le 0.01} \Theta(t) = \Theta(0.01) = 0.028513162 \cdots$$

Thus, combining the above with (3.46) yields

$$|a_1'(t)| \le 8\pi^3\Theta(0.01)\exp(13t - \pi e^{4t}) \qquad (0 \le t \le 0.01).$$

Now, using (3.47) and the upper bound for $|\Phi'_1(t)|$ in (3.12) of Lemma 3.3, we have from (3.45) that

(3.48)
$$3|\Phi'(t)\Phi(t)| \le 3(1.087872648)\pi^{5}\exp(22t - 2\pi e^{4t})$$
$$\times \left[8\Theta(0.01) + 565\exp(-3\pi e^{4t})\right]$$

for $t_0 \le t \le 0.01$. Now, the quantity in brackets above is strictly decreasing for all $t \ge 0$, the same being true for the factor $\exp(22t - 2\pi e^{4t})$. Thus, the maximum of the right side of (3.48), for $0 \le t \le 0.01$, is taken on at $t = t_0$, which gives

$$(3.49) 3|\Phi'(t)\Phi(t)| \le 0.505\,076\,975 < 0.506 (0 \le t \le 0.01).$$

Combining the above with (3.44) gives the desired result of (3.38). \Box

LEMMA 3.9. With the definition of g(t) in (3.26),

$$(3.50) g(t) > 0 (0 < t \le 0.01).$$

PROOF. To establish (3.50), it suffices, from (3.23), to show that (cf. (3.24))

(3.51)
$$g'(0) + \frac{g^{(2)}(\xi)t}{2} > 0 \qquad (\xi \in (0, t); 0 < t \le 0.01).$$

Now, by (3.25), we have that

$$g^{(2)}(t) = 3\Phi'(t)\Phi(t) + t[\Phi(t)]^2 + J(t)\Phi^{(3)}(t).$$

Since J(t) > 0 for all $t \ge 0$ from (3.17), and since $\Phi^{(3)}(t) > 0$ for $0 < t \le 0.01$ from (3.33) of Lemma 3.7, it follows that, with (i) and (v) of Theorem A,

$$g^{(2)}(t) \geqslant 3\Phi'(t)\Phi(t) = -3|\Phi'(t)\Phi(t)| \qquad (0 \leqslant t \leqslant 0.01).$$

Hence, from (3.38) of Lemma 3.8,

$$(3.52) g^{(2)}(t) \ge -0.506 (0 \le t \le 0.01).$$

On the other hand, by (3.29) of Lemma 3.6, g'(0) > 0.018790453. Thus, with (3.52),

$$g'(0) + \frac{g^{(2)}(\xi)t}{2} \ge 0.018790453 + \frac{0.01}{2}(-0.506),$$

or

$$g'(0) + \frac{g^{(2)}(\xi)t}{2} \ge 0.016260453$$
 $(0 \le t \le 0.01),$

which establishes (3.51). \square

It is still necessary to show that g(t), defined in (3.26), is positive for all $t \ge 0.01$. To this end, we decompose g(t) as

$$(3.53) g(t) = G_1(t) + G_2(t),$$

where

$$(3.54) G_1(t) := J(t)a_1'(t) + ta_1^2(t),$$

and where

(3.55)
$$G_2(t) := J(t)\Phi_1'(t) + 2ta_1(t)\Phi_1(t) + [\Phi_1(t)]^2.$$

Our next immediate goal is to provide bounds for $G_1(t)$ and $G_2(t)$.

LEMMA 3.10. Set

(3.56)
$$E_1(t) := \pi^2 \exp(10t - 2\pi e^{4t}) \Psi_1(t),$$

where

(3.57)
$$\Psi_1(t) := \pi e^{4t} (3t - 1) + \frac{3t}{2} + \frac{15}{4} - \frac{15}{8\pi e^{4t}}.$$

Then (cf. (3.54)),

(3.58)
$$G_1(t) \geqslant E_1(t) \quad (t \geqslant 0.01).$$

PROOF. From (vii) of Theorem A, we have that $a_1'(t) < 0$ for all $t > t_0$, where (cf. (1.15)) $t_0 = 0.00011334 \cdots$. Thus, from the definition of $G_1(t)$ in (3.54) and from (3.18) of Lemma 3.5,

$$(3.59) \quad G_1(t) \geqslant \left(\frac{\pi t}{2} + \frac{e^{-4t}}{8}\right) \exp(5t - \pi e^{4t}) \cdot a_1'(t) + t a_1^2(t) \qquad (t > t_0).$$

On substituting the definition of $a_1(t)$ (cf. (3.1)) in the right side of (3.59) and simplifying, the right side of (3.59) reduces exactly to $E_1(t)$ of (3.56). As $t_0 < 0.01$, (3.58) is then evidently satisfied. \square

LEMMA 3.11. Set

(3.60)
$$E_2(t) := \pi^2 \exp(10t - 2\pi e^{4t}) \Psi_2(t),$$

where

(3.61)
$$\Psi_2(t) := \exp(8t - 3\pi e^{4t}) \left(-223.6\pi^2 t - \frac{565\pi}{8e^{4t}} \right).$$

Then (cf. (3.53)),

(3.62)
$$G_2(t) > E_2(t) \quad (t \ge 0).$$

PROOF. Since $a_n(t) > 0$ for all $t \ge 0$ and for each $n \ge 1$ from (i) of Theorem A, then $\Phi_1(t) > a_2(t)$ for all $t \ge 0$ from (3.3). Hence (cf. (3.55)),

(3.63)
$$G_2(t) > J(t)\Phi_1'(t) + 2ta_1(t)a_2(t) \qquad (t \ge 0).$$

Since J(t) > 0 from (3.17), for all $t \ge 0$, and since $\Phi'_1(t) < 0$ from (3.3) and (vi) of Theorem A, for all $t \ge 0$, then by (3.12) of Lemma 3.3 and (3.17) of Lemma 3.5, we have

$$J(t)\Phi_1'(t) \ge -565\pi^3 \left(\frac{\pi t}{2} + \frac{e^{-4t}}{8}\right) \exp(18t - 5\pi e^{4t}) \qquad (t \ge 0).$$

Also, from (3.1), we have

$$2ta_1(t)a_2(t) = 16\pi^2t(2\pi e^{4t} - 3)(8\pi e^{4t} - 3)\exp(10t - 5\pi e^{4t}).$$

Substituting the above two expressions into (3.63) and simplifying then gives

$$G_2(t) > \pi^4 \exp(18t - 5\pi e^{4t}) \left\{ -223.6t - \frac{565}{8\pi e^{4t}} \right\},$$

which, from the definitions of (3.60) and (3.61), is the desired result of (3.62). \Box This brings us to the final result of this section, namely

LEMMA 3.12. With the definition of g(t) in (3.26), then

$$(3.64) g(t) > 0 (t > 0).$$

PROOF. If $0 < t \le 0.01$, then g(t) > 0 by (3.50) of Lemma 3.9. Then, it suffices to consider only $t \ge 0.01$. Then, from (3.53) and Lemmas 3.10 and 3.11, we have

$$g(t) \ge E_1(t) + E_2(t)$$
 $(t \ge 0.01)$,

which, from (3.56) and (3.60), can be equivalently expressed as

(3.65)
$$g(t) \ge \pi^2 \exp(10t - 2\pi e^{4t}) \Psi(t) \qquad (t \ge 0.01),$$

where

(3.66)
$$\Psi(t) := \Psi_1(t) + \Psi_2(t).$$

From (3.57) and (3.61), we verify that

(3.67)
$$\Psi_1'(t) = \pi e^{4t} (12t - 1) + \frac{3}{2} + \frac{15}{2\pi e^{4t}},$$

and that

(3.68)

$$\Psi_2'(t) = \exp(8t - 3\pi e^{4t}) \left\langle \pi^2 t (2683.2\pi e^{4t} - 1788.8) + \pi \left(623.9\pi - \frac{565}{2e^{4t}}\right) \right\rangle.$$

It is clear from (3.68) that $\Psi_2'(t) > 0$ for all $t \ge 0$. Similarly, we claim that $\Psi_1'(t) > 0$ for all $t \ge 0$. First, from (3.67), we see that $\Psi_1'(0) = 0.74573 \cdots > 0$, and that

$$\Psi_1^{(2)}(t) = 48\pi t e^{4t} + 8\pi e^{4t} - \frac{30}{\pi e^{4t}},$$

so that $\Psi_1^{(2)}(t) > 0$ for all $t \ge 0$. Hence, $\Psi_1'(t) > 0$ for all $t \ge 0$. Thus, from (3.66), $\Psi(t)$ is strictly increasing for $t \ge 0$, with

and we conclude from (3.65) that

(3.69)
$$g(t) \ge \pi^2 \exp(10t - 2\pi e^{4t}) \Psi(t) > 0 \qquad (t \ge 0.01),$$

which gives the desired inequality (3.64). \Box

We remark that the function $\Psi(t)$ of (3.66) is, in fact, negative for $0 \le t \le 0.005$, which supports the necessity of separately considering the two intervals $0 \le t \le 0.01$ and $t \ge 0.01$ in the proof of Lemma 3.12.

4. Numerical computation of moments and Turán differences. The accurate calculation of the moments \hat{b}_m (m = 0, 1, 2, ...) of (1.5) involves two separate numerical problems. First, from (1.3), we can express $\Phi(t)$ of (1.3) in the form

$$\Phi(t) = \sum_{n=1}^{\infty} a(n,t),$$

where (cf. (1.14))

$$(4.2) a(x,t) := (2\pi^2 x^4 e^{9t} - 3\pi x^2 e^{5t}) \exp(-\pi x^2 e^{4t}).$$

As in (i) of Theorem A, it is readily verified that

$$(4.3) a(x,t) > 0 (x \ge 1, t \ge 0),$$

and that

$$\frac{\partial a(x,t)}{\partial x} < 0 \quad (x \ge 1, t \ge 0).$$

Because of (4.4), the integral test gives that

(4.5)
$$0 < \Phi(t) - \sum_{n=1}^{N} a(n,t) < \int_{N}^{\infty} a(x,t) dx.$$

Moreover, it can be verified (after an integration by parts) that

$$\int_{N}^{\infty} a(x,t) dx = \pi N^{3} \exp(5t - \pi N^{2}e^{4t}),$$

so that (4.5) becomes

(4.6)
$$0 < \Phi(t) - \sum_{n=1}^{N} a(n,t) < \pi N^3 \exp(5t - \pi N^2 e^{4t}).$$

The above upper bound for the error, in approximating $\Phi(t)$ by its partial sum of N terms, turns out to be quite accurate.

Next, for the moments \hat{b}_m of (1.5), we write

$$\hat{b}_m := \int_0^\infty t^{2m} \Phi(t) dt = \int_0^1 t^{2m} \Phi(t) dt + \int_1^\infty t^{2m} \Phi(t) dt,$$

or

(4.7)
$$\hat{b}_m = \int_0^1 t^{2m} \Phi(t) dt + \int_0^1 u^{-(2m+2)} \Phi\left(\frac{1}{u}\right) du \qquad (m = 0, 1, \dots).$$

Because of the exponential decay to zero of $\Phi(t)$ as $t \to \infty$, the singularity at u = 0 in the last integral of (4.7) is removable for each $m \ge 0$.

The numerical procedure used for calculating the moments \hat{b}_m was the following. The two integrals in (4.7) were each approximated numerically by Romberg integration (cf. Stoer and Bulirsch [SB, p. 132]), where $\Phi(t)$ was approximated by the finite sum in (4.6). The iteration in Romberg integration was continued (for each integral in (4.7)) until two entries in a single column agreed to sixty decimal digits. For the values $\Phi(t)$ of the integrands of the integrals in (4.7), the associated number N (of the terms of the finite sum approximation to $\Phi(t)$ was selected so that the approximation error in (4.6) was less than 10⁻⁶⁰. The computations were performed in FORTRAN 77, using Richard Brent's MP package (cf. Brent [Br]) for extendedprecision floating-point numbers and 110 digits of precision, on a VAX-11/780 in the Department of Mathematical Sciences at Kent State University. The absolute error in computing the moments $\{\hat{b}_m\}_{m=0}^{20}$ was less than 10^{-50} in all cases. While it appears from Table 4.1 that the moments \hat{b}_m are decreasing quite rapidly, we mention the fact that they are eventually increasing. (The details of this will appear elsewhere.) The relative error of these moments $\{\hat{b}_m\}_{m=0}^{20}$ was less than 10^{-40} in all cases.

Though only the first three moments $\{\hat{b}_m\}_{m=0}^2$ were specifically needed in §2 to complete the proof of Theorem 2.5, it was thought that a lengthier tabulation of these moments might be of interest to the reader, particularly since such a tabulation of these moments does not exist in the literature. Although the moments $\{\hat{b}_m\}_{m=0}^{109}$ were actually numerically determined, we have, for the sake of brevity, included in Table 4.1 only the moments $\{\hat{b}_m\}_{m=0}^{20}$, here rounded to sixteen significant digits. Also included in this table are the associated Turán differences $\{D_m\}_{m=1}^{19}$, where

(4.8)
$$D_m := (\hat{b}_m)^2 - \left(\frac{2m-1}{2m+1}\right)\hat{b}_{m-1}\hat{b}_{m+1} \qquad (m=1,2,\ldots).$$

Table 4.1

| m | \hat{b}_m | D_m |
|----|-----------------------------|-----------------------------|
| 0 | 6.214 009 727 353 926 (-2) | |
| 1 | 7.178 732 598 482 949 (-4) | 3.588 449 148 619 957 (-8) |
| 2 | 2.314 725 338 818 463 (-5) | 3.163 299 395 056 600 (-11) |
| 3 | 1.170 499 895 698 397 (-6) | 7.056 732 441 900 485 (-14) |
| 4 | 7.859 696 022 958 770 (-8) | 2.832 220 223 070 768 (-16) |
| 5 | 6.474 442 660 924 152 (-9) | 1.736 366 689 470 613 (-18) |
| 6 | 6.248 509 280 628 118 (-10) | 1.478 031 720 106 092 (-20) |
| 7 | 6.857 113 566 031 334 (-11) | 1.641 533 684 538 624 (-22) |
| 8 | 8.379 562 856 498 463 (-12) | 2.277 443 847 755 004 (-24) |
| 9 | 1.122 895 900 525 652 (-12) | 3.822 737 726 048 953 (-26) |
| 10 | 1.630 766 572 462 173 (-13) | 7.575 377 587 713 463 (-28) |
| 11 | 2.543 075 058 368 090 (-14) | 1.738 493 426 852 891 (-29) |
| 12 | 4.226 693 865 498 318 (-15) | 4.549 255 646 782 005 (-31) |
| 13 | 7.441 357 184 567 353 (-16) | 1.340 195 434 809 036 (-32) |
| 14 | 1.380 660 423 385 153 (-16) | 4.397 768 675 764 370 (-34) |
| 15 | 2.687 936 596 475 912 (-17) | 1.593 011 938 279 461 (-35) |
| 16 | 5.470 564 386 990 504 (-18) | 6.320 855 730 991 445 (-37) |
| 17 | 1.160 183 185 841 992 (-18) | 2.728 993 526 800 843 (-38) |
| 18 | 2.556 698 594 979 872 (-19) | 1.274 579 325 080 585 (-39) |
| 19 | 5.840 019 662 344 811 (-20) | 6.406 797 431 277 575 (-41) |
| 20 | 1.379 672 872 080 269 (-20) | |

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