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Orthogonal polynomial expansions for the Riemann xi function in the Hermite, Meixner–Pollaczek, and continuous Hahn bases

by

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Contents

1. Introduction

1.1. Background. This paper concerns the study of certain infinite series expansions for the Riemann xi function $\xi(s)$. Recall that $\xi(s)$ is defined in terms of Riemann's zeta function $\zeta(s)$ by

$$\xi(s) = \tfrac{1}{2}s(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s) \quad (s \in \mathbb{C}). \tag{1.1}$$

The function $\xi(s)$ is entire and satisfies the functional equation

$$\xi(1-s) = \xi(s). \tag{1.2}$$

It is convenient and customary to perform a change of variables, denoting

$$\Xi(t) = \xi(1/2 + it) \quad (t \in \mathbb{C}), \tag{1.3}$$

a function that (in keeping with convention) will also be referred to as the Riemann xi function. The functional equation (1.2) then becomes the statement that $\Xi(t)$ is an even function. The xi function has been a key tool

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in the study of the complex-analytic properties of $\zeta(s)$ and, crucially, the Riemann Hypothesis (RH). Two additional standard properties of $\Xi(t)$ are that it takes real values on the real line, and that RH can be stated as the claim that all the zeros of $\Xi(t)$ are real [64].

1.1.1. *Some representations of the Riemann xi function.* Much research on the zeta function has been based on studying various series and integral representations of $\zeta(s)$, $\xi(s)$ and $\Xi(t)$, in the hope that this might provide information about the location of their zeros. For example, it is natural to investigate the sequence of coefficients in the Taylor expansion

$$\xi(s) = \sum_{n=0}^{\infty} a_{2n}(s-1/2)^{2n}. \tag{1.4}$$

Riemann himself derived in his seminal 1859 paper a formula for the coefficients a_{2n} (see [21, p. 17]), which in our notation reads as

$$a_{2n} = \frac{1}{2^{2n-1}(2n)!}\int_1^{\infty} \omega(x)x^{-3/4}(\log x)^{2n}\,dx \tag{1.5}$$

(where $\omega(x)$ is defined below in (1.7)), and which plays a small role in the theory. The study of the numbers a_{2n} remains an active area of research [14, 16, 22, 55, 56, 57]—we also discuss them in Section 5—but, disappointingly, the Taylor expansion (1.4) has not provided much insight into the location of the zeros of $\zeta(s)$.

Another important way to represent $\xi(s)$, also considered by Riemann, is as a Mellin transform, or—which is equivalent through a standard change of variables—as a Fourier transform. Define functions $\theta(x), \omega(x), \Phi(x)$ by

$$\theta(x) = \sum_{n=-\infty}^{\infty} e^{-\pi n^2 x} = 1 + 2\sum_{n=1}^{\infty} e^{-\pi n^2 x} \qquad (x>0), \tag{1.6}$$

$$\begin{aligned}\omega(x) &= \tfrac{1}{2}(2x^2\theta''(x) + 3x\theta'(x)) \\ &= \sum_{n=1}^{\infty}(2\pi^2 n^4 x^2 - 3\pi n^2 x)e^{-\pi n^2 x} \qquad (x>0),\end{aligned} \tag{1.7}$$

$$\begin{aligned}\Phi(x) &= 2e^{x/2}\omega(e^{2x}) \\ &= 2\sum_{n=1}^{\infty}(2\pi^2 n^4 e^{9x/2} - 3\pi n^2 e^{5x/2})\exp(-\pi n^2 e^{2x}) \qquad (x\in\mathbb{R}).\end{aligned} \tag{1.8}$$

Then it is well-known that $\theta(x), \omega(x), \Phi(x)$ are positive functions, satisfy the functional equations (all equivalent to each other, as well as to (1.2))

$$\theta\left(\frac{1}{x}\right) = \sqrt{x}\,\theta(x), \qquad \omega\left(\frac{1}{x}\right) = \sqrt{x}\,\omega(x), \qquad \Phi(-x) = \Phi(x), \tag{1.9}$$

and that $\xi(s)$ has the Mellin transform representation

$$\xi(s) = \int_0^\infty \omega(x) x^{s/2-1}\, dx, \tag{1.10}$$

and the Fourier transform representation

$$\Xi(t) = \int_{-\infty}^\infty \Phi(x) e^{itx}\, dx. \tag{1.11}$$

The right-hand side of (1.11) is also frequently written in equivalent form as a cosine transform, that is, replacing the e^{itx} term with $\cos(tx)$, which is valid since $\Phi(x)$ is an even function. For additional background, see [21, 64].

1.1.2. *Pólya's attack on RH and its offshoots by de Bruijn, Newman and others.* Pólya in the 1920s began an ambitious line of attack on RH in a series of papers [49, 50, 51, 52] (see also [64, Ch. X]) in which he investigated sufficient conditions for an entire function represented as the Fourier transform of a positive even function to have all its zeros lie on the real line. Pólya's ideas have been quite influential and found important applications in areas such as statistical physics (see [37], [39], [53, pp. 424–426]). One particular result that proved consequential is Pólya's discovery that the factor $e^{\lambda x^2}$, where $\lambda > 0$ is constant, is (to use a term apparently coined by de Bruijn [10]) a so-called *universal factor*. That is to say, Pólya's theorem states that if an entire function $G(z)$ is expressed as the Fourier transform of a function $F(x)$ of a real variable, and all the zeros of $G(z)$ are real, then, under certain assumptions of rapid decay on $F(x)$ (see [10] for details), the zeros of the Fourier transform of $F(x)e^{\lambda x^2}$ are also all real. This discovery spurred much follow-up work by de Bruijn [10], Newman [38] and others [17, 18, 19, 20, 31, 40, 41, 54, 59, 60, 58] on the subject of what came to be referred to as the *de Bruijn–Newman constant*; the rough idea is to launch an attack on RH by generalizing the Fourier transform (1.11) through the addition of the "universal factor" $e^{\lambda x^2}$ inside the integral, and to study the set of real λ's for which the resulting entire function has only real zeros. See Section 2.5, where some additional details are discussed, and see [9, Ch. 5], [39] for accessible overviews of the subject.

1.1.3. *Turán's approach.* Next, we survey another attack on RH that is the closest one conceptually to our current work, proposed by Pál Turán. In a 1950 address to the Hungarian Academy of Sciences [66] and follow-up papers [67, 68], Turán took a novel look at the problem, starting by re-examining the idea of looking at the Taylor expansion (1.4) and then analyzing why it fails to lead to useful insights and how one might try to improve on it. He argued that the coefficients in the Taylor expansion of an entire function provide the wrong sort of information about the zeros of the function, being in general well-suited for estimating the distance of the zeros from the origin, but poorly adapted for the purpose of telling whether the zeros lie on the real line. As a heuristic explanation, he pointed out that the level curves of the power functions $z \mapsto z^n$ are concentric circles, and argued that one must therefore look instead for series expansions of the Riemann xi function in functions whose level curves approximate straight lines running parallel to the real axis. He then argued that the Hermite polynomials

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2})$$

are such a family of functions, and proceeded to proving several results demonstrating his main thesis that the coefficients in the Fourier series expansion of a function in Hermite polynomials can in many cases provide useful information about the distance of the zeros of the function from the real line.

Turán also made the important observation that the expansion of $\varXi(t)$ in Hermite polynomials has a rather nice structure, being expressible in the form

$$\varXi(t) = \sum_{n=0}^{\infty} (-1)^n b_{2n} H_{2n}(t) \tag{1.12}$$

in which, he pointed out, the coefficients b_{2n} are given by the formula ([1])

$$b_{2n} = \frac{1}{2^{2n}(2n)!} \int_{-\infty}^{\infty} x^{2n} e^{-x^2/4} \varPhi(x)\, dx, \tag{1.13}$$

and in particular are positive numbers.

Note that the Hermite polynomials satisfy the symmetry $H_n(-x) = (-1)^n H_n(x)$, so, as in the case of the Taylor expansion (1.4), the presence of only even-indexed coefficients in (1.12) is a manifestation of the functional equation (1.9), and hence serves as another indication that the expansion (1.12) is a somewhat natural one to consider. (Of course, the same would be true for any other family of even functions; this is obviously a weak criterion for naturalness.)

Turán focused most of his attention on Hermite expansions of polynomials rather than of entire functions like $\varXi(t)$. His ideas on locating polynomial zeros using knowledge of the coefficients in their Hermite expansions appear to have been quite influential, and have inspired many subsequent fruitful investigations into the relationship between the expansion of a polynomial in Hermite polynomials and other orthogonal polynomial families, and the location of the zeros of the polynomial. See the papers [7, 8, 25, 26, 27, 28, 47, 61].

([1]) Actually Turán's formula in [68] appears to contain a small numerical error, differing from (1.13) by a factor of $\pi/2$.

By contrast, Turán's specific observation about the expansion (1.12) of $\Xi(t)$ does not seem to have led to any meaningful follow-up work. We are not aware of any studies of the behavior of the coefficients b_{2n}, nor of any attempts to determine whether the Hermite polynomials are the only—or even the most natural—family of polynomials in which it is worthwhile to expand the Riemann xi function (but see Section 1.3 for discussion of some related literature).

1.2. Our new results: Turán's program revisited and extended; expansion of $\Xi(t)$ in new orthogonal polynomial bases. This paper can be thought of as a natural continuation of the program of research initiated by Turán in his 1950 address. One direction we pursue is a renewed analysis of the Hermite expansion (1.12) introduced by Turán in which we answer several questions that were left unaddressed by him. For example, in Theorem 2.7 we derive an asymptotic formula for the coefficients b_{2n}. We will also show a previously unnoticed connection between Turán's ideas on the Hermite expansion and the separate thread of research on the topic of the de Bruijn–Newman constant described in the previous section. The idea is that the so-called Pólya–de Bruijn flow—the one-parameter family of approximations to the Riemann xi function obtained by introducing the factor $e^{\lambda x^2}$ to the Fourier transform in (1.11)—shows up in a natural way also when taking the Hermite expansion (1.12) and using it to separately construct a family of approximations inspired by the standard construction of Poisson kernels in the theory of orthogonal polynomials.

Going beyond the Hermite expansion, we will explore the possibility that Turán's vision of understanding the Riemann xi function by studying its expansion in the Hermite polynomials was too narrow in its scope. More precisely, it turns out that there is a wealth of new and interesting results related to the notion of expanding $\Xi(t)$ in *different* families of orthogonal polynomials. Two very specific orthogonal polynomial families appear to suggest themselves as being especially natural and possessve of good properties. Those are the *Meixner–Pollaczek polynomials* $P_n^{(\lambda)}(x;\phi)$ with the specific parameter values $\phi = \pi/2$, $\lambda = 3/4$, and the *continuous Hahn polynomials* $p_n(x;a,b,c,d)$ with the specific parameter values $a = b = c = d = 3/4$. We denote these families of polynomials by $(f_n)_{n=0}^{\infty}$ and $(g_n)_{n=0}^{\infty}$, respectively; they are given explicitly by the hypergeometric formulas

$$f_n(x) = \frac{(3/2)_n}{n!} i^n \, {}_2F_1\left(-n, \frac{3}{4} + ix; \frac{3}{2}; 2\right), \tag{1.14}$$

$$g_n(x) = i^n (n+1) \, {}_3F_2\left(-n, n+2, \frac{3}{4} + ix; \frac{3}{2}, \frac{3}{2}; 1\right) \tag{1.15}$$

(where $(3/2)_n$ is a Pochhammer symbol), and form systems of polynomials that are orthogonal with respect to the weight functions $|\Gamma(3/4+ix)|^2$ and $|\Gamma(3/4+ix)|^4$ on $\mathbb{R}$, respectively.

As our analysis will show, the expansions of $\Xi(t)$ in the polynomial families $(f_n)_{n=0}^\infty$ and $(g_n)_{n=0}^\infty$ have forms that are pleasingly similar to the Hermite expansion (1.12), namely

$$\Xi(t) = \sum_{n=0}^\infty (-1)^n c_{2n} f_{2n}\left(\frac{t}{2}\right), \tag{1.16}$$

$$\Xi(t) = \sum_{n=0}^\infty (-1)^n d_{2n} g_{2n}\left(\frac{t}{2}\right), \tag{1.17}$$

where, importantly, the coefficients c_{2n} and d_{2n} again turn out to be positive numbers. Moreover, we will investigate the rather subtle connections between the two expansions (1.16)–(1.17), and prove that the coefficients c_{2n} and d_{2n} satisfy the two asymptotic formulas

$$c_{2n} \sim 16\sqrt{2}\,\pi^{3/2}\sqrt{n}\,\exp(-4\sqrt{\pi n}), \tag{1.18}$$

$$d_{2n} \sim \left(\frac{128\times 2^{1/3}\pi^{2/3}e^{-2\pi/3}}{\sqrt{3}}\right) n^{4/3}\exp(-3(4\pi)^{1/3}n^{2/3}) \tag{1.19}$$

as $n\to\infty$. See Theorems 3.2 and 4.3 for precise statements, including explicit rate of convergence estimates.

Significance of the new expansions. Turán's attack on the Riemann Hypothesis was not successful, yet opened up new and interesting avenues of research into the Riemann zeta function and the study of complex polynomials and their zeros. Our new results similarly have not yielded us new information on the location of the zeros of $\Xi(t)$. Thus, if the present work is regarded as an attack on RH, it is a failed one at worst, or a still-speculative one at best (of course, in our defense the same can doubtlessly be said of all other attacks on RH to date). Given such an uncertain state of affairs, one might ask why the polynomial bases $(f_n)_{n=0}^\infty$ and $(g_n)_{n=0}^\infty$ deserve special attention as bases in which to expand $\Xi(t)$, as compared to the Hermite polynomials or any other orthogonal polynomial family; and in particular, whether the expansions in these particular bases hold any more promise of revealing some fundamental new insights into the location of the zeros than other expansions.

One possible answer is that the two weight functions $|\Gamma(3/4+ix)|^2$ and $|\Gamma(3/4+ix)|^4$ appearing in the orthogonality relations for these orthogonal polynomial families seem more adapted to the analytic-number-theoretic nature of $\Xi(t)$, being specifically tied to the gamma-factor appearing in the definition (1.1) of $\xi(s)$; this is in contrast to the somewhat arbitrary-looking weight function e^{-x^2}. Another hint of naturalness of the two new bases is that the positivity of the coefficients c_{2n} and d_{2n} is an unusual property that is enjoyed as well by the coefficients for the Hermite expansion, but which will not hold for a generic orthogonal polynomial expansion (note for example that for our results it is essential to use the particular variable scaling $f_{2n}(t/2)$ and $g_{2n}(t/2)$ in (1.16)–(1.17); if a different scaling $f_{2n}(\beta t)$ and $g_{2n}(\beta t)$ were to be used for some arbitrary scaling parameter β, there is no reason to expect a particular pattern of signs for the coefficients).

Perhaps the most compelling answer ultimately lies in the results themselves which we will prove about the two new expansions: the elegance of the formulas for the coefficients and their asymptotics, and of the analysis leading to those formulas, suggests that the expansions (1.16)–(1.17) are simply a natural structure that is worthy of being studied and understood, both for its own sake and for potential applications to RH and other open problems in the theory of the Riemann zeta function.

See also Remark (1) in Section 6 for some related thoughts on the potential benefits of studying the expansions (1.16)–(1.17), and orthogonal polynomial expansions of $\Xi(t)$ in general.

1.3. Previous work involving the polynomials f_n. Our work on the Hermite expansion of the Riemann xi function is, as mentioned above, a natural continuation of Turán's work, and also relates to the existing literature on the de Bruijn–Newman constant. By contrast, our results on the expansion of the Riemann xi function in the polynomial families f_n and g_n in Sections 3–4 do not appear to follow up on any established line of research. It seems worth mentioning however that the polynomials f_n did in fact make an appearance in a few earlier works in contexts involving the Riemann zeta and xi functions.

The earliest such work we are aware of is the paper by Bump and Ng [12], which discusses polynomials that are (up to a trivial reparametrization) the polynomials f_n in connection with some Mellin transform calculations related to the zeta function. The follow-up papers by Bump et al. [11] and Kurlberg [34] discuss these polynomials further, in particular interpreting their property of having only real zeros in terms of a phenomenon that the authors term the "local Riemann Hypothesis". The idea of using these polynomials as a basis in which to expand the Riemann xi function (or any other function) does not appear in these papers, but they seem nonetheless to be the first works that contain hints that the polynomials f_n may hold some significance for analytic number theory.

In another paper [36] (see also [35]), Kuznetsov actually does consider an expansion in the polynomial basis $f_n(t/2)$—the same basis we use for our expansion of $\Xi(t)$—of a modified version of the Riemann xi function, namely the function $e^{-\pi t/4}\Xi(t)$, and finds formulas for the coefficients in the expansion in terms of the Taylor coefficients of an elementary function. Kuznetsov's result gives yet more clues as to the special role played in the theory of the Riemann xi function by the polynomials f_n. It is however unclear to us how his results relate to ours.

Finally, in a related direction, Inoue, apparently motivated by the work of Kuznetsov, studies in a recent preprint [24] the expansion of the completed zeta function $\pi^{-s/2}\Gamma(s/2)\zeta(s)$ in the polynomials $f_n(t/2)$, and proves convergence of the expansion in the critical strip.

1.4. Structure of the paper. The main part of this paper consists of Sections 2–4. These sections are arranged in two conceptually distinct parts: Section 2, which deals with the Hermite expansion of the Riemann xi function and its connection to the de Bruijn–Newman constant, forms the first part; and Sections 3–4, which develop the theory of the expansion of the Riemann xi function in the orthogonal polynomial families $(f_n)_{n=0}^\infty$ and $(g_n)_{n=0}^\infty$, form the second. The second part is largely independent of the first, so it would be practical for the reader to start reading directly from Section 3 and only refer back to Section 2 as needed on a few occasions.

In Section 5 we prove an asymptotic formula for the Taylor coefficients of $\Xi(t)$, and conclude in Section 6 with some final remarks.

The work makes heavy use of known properties of several families of orthogonal polynomials. The Appendix summarizes the relevant properties, and ends with a section in which we prove a new pair of identities relating the polynomial families $(f_n)_{n=0}^\infty$ and $(g_n)_{n=0}^\infty$.

We assume the reader is familiar with the basic theory of orthogonal polynomials, as described, e.g., in Chapters 2–3 of Szegő's classical book [63] on the subject. We also assume familiarity with standard special functions such as the Euler gamma function $\Gamma(s)$ and Gauss hypergeometric function ${}_2F_1(a,b;c;z)$ (see [1]), and of course with basic results and facts about the Riemann zeta function [21]. For background on Mellin transforms, of which we make extensive use, the reader is invited to refer to [42].

2. The Hermite expansion of $\Xi(t)$. The goal of this section is to expand on Turán's work in [66, 67, 68] on the series expansion of $\Xi(t)$ in Hermite polynomials. In Section 2.1 we state a precise version of Turán's claims about the existence of the expansion, showing that it holds on the entire complex plane and giving a quantitative rate of convergence estimate. This is proved in Section 2.3. In Section 2.4 we prove an asymptotic formula for the coefficients b_{2n} appearing in the expansion. In Section 2.5 we show how the Hermite expansion leads naturally to a one-parameter family of approximations to the Riemann xi function, which we will show is (up to a trivial transformation) the same family studied in the works of de

Bruijn, Newman and subsequent authors on what came to be known as the de Bruijn–Newman constant.

2.1. The basic convergence result for the Hermite expansion. Following Turán [68], we define numbers $(b_n)_{n=0}^{\infty}$ by

$$b_n = \frac{1}{2^n n!} \int_{-\infty}^{\infty} x^n e^{-x^2/4} \Phi(x)\, dx \tag{2.1}$$

with $\Phi(x)$ defined in (1.8). Since $\Phi(x)$ is even and positive, we see that $b_{2n+1} = 0$ and $b_{2n} > 0$ for all $n \geq 0$. The following result is a more precise version of Turán's remarks in [66] about the expansion of $\Xi(t)$ in Hermite polynomials.

THEOREM 2.1 (Hermite expansion of $\Xi(t)$). *The Riemann xi function has the infinite series representation*

$$\Xi(t) = \sum_{n=0}^{\infty} (-1)^n b_{2n} H_{2n}(t), \tag{2.2}$$

which converges uniformly on compacts for all $t \in \mathbb{C}$. More precisely, for any compact set $K \subset \mathbb{C}$ there exist constants $C_1, C_2 > 0$ depending on K such that

$$\Big| \Xi(t) - \sum_{n=0}^{N} (-1)^n b_{2n} H_{2n}(t) \Big| \leq C_1 e^{-C_2 N \log N} \tag{2.3}$$

for all $N \geq 1$ and $t \in K$.

We note for the record the unsurprising fact that the coefficients b_{2n} can also be computed as the Fourier coefficients of $\Xi(t)$ associated with the orthonormal basis of Hermite polynomials in the function space $L^2(\mathbb{R}, e^{-t^2} dt)$.

COROLLARY 2.2. *An alternative expression for the coefficients b_{2n} is*

$$b_{2n} = \frac{(-1)^n}{\sqrt{\pi}\, 2^{2n} (2n)!} \int_{-\infty}^{\infty} \Xi(t) e^{-t^2} H_{2n}(t)\, dt. \tag{2.4}$$

We give the easy proof of Corollary 2.2 at the end of Section 2.3 following the proof of Theorem 2.1.

2.2. Preliminaries. Recall the easy fact that the series (1.7)–(1.8) defining $\omega(x)$ and $\Phi(x)$ are asymptotically dominated by their first summands as $x \to \infty$, and that this remains true if the series are summed starting at $m = 2$. This leads to the following standard estimates (with the second one also relying on (1.9)), which will be used several times in this and the following sections.

Lemma 2.3. *The functions* $\omega(x)$ *and* $\Phi(x)$ *satisfy the asymptotic estimates*

$$\omega(x) = O(x^2 e^{-\pi x}) \qquad \text{as } x \to \infty, \tag{2.5}$$

$$\omega(x) = O(x^{-5/2} e^{-\pi/x}) \qquad \text{as } x \to 0+, \tag{2.6}$$

$$\omega(x) - (2\pi^2 x^2 - 3\pi x)e^{-\pi x} = O(x^2 e^{-4\pi x}) \qquad \text{as } x \to \infty, \tag{2.7}$$

$$\Phi(x) = O(\exp(9x/2 - \pi e^{2x})) \qquad \text{as } x \to \infty, \tag{2.8}$$

$$\begin{aligned}\Phi(x) - 2(2\pi^2 e^{9x/2} - 3\pi e^{5x/2}) \exp(-\pi e^{2x}) \\ = O(\exp(9x/2 - 4\pi e^{2x})) \qquad \text{as } x \to \infty.\end{aligned} \tag{2.9}$$

2.3. Proof of Theorem 2.1. We start by stating an easy (and far from sharp, but sufficient for our purposes) bound on the rate of growth of $H_n(t)$ as a function of n.

Lemma 2.4. *The Hermite polynomials satisfy the bound*

$$|H_n(t)| \le C \exp\left(\tfrac{3}{4} n \log n\right) \tag{2.10}$$

for all $n \ge 1$*, uniformly as* t *ranges over any compact set* $K \subset \mathbb{C}$*, with* $C > 0$ *being a constant that depends on* K *but not on* n*.*

Proof. This is immediate from the well-known asymptotic expansion for the Hermite polynomials; see [63, p. 200, Th. 8.22.7]. ■

Define the *Lambert* W*-function* to be the unique increasing function $W : [0, \infty) \to [0, \infty)$ satisfying the equation

$$W(xe^x) = x.$$

In what follows, we will make use of the following asymptotic formula for $W(x)$ for large x. The result is a weaker version of [15, eq. (4.19)].

Theorem 2.5 (Corless et al. [15]). *The asymptotic behavior of* $W(x)$ *as* $x \to \infty$ *is given by*

$$W(x) = \log x - \log\log x + \frac{\log\log x}{\log x} + O\left(\left(\frac{\log\log x}{\log x}\right)^2\right). \tag{2.11}$$

The Lambert W-function and its asymptotics will be quite important for our analysis. A hint of why this is so can already be glimpsed in the proof of the following technical lemma.

Lemma 2.6. *For any number* $B \ge 1$ *there is a constant* $C > 0$ *such that*

$$\begin{aligned}&\int_0^\infty x^n \exp(-Be^x)\, dx \\ &\quad \le \exp\left[n \log\log n - \frac{n \log\log n}{\log n} - (\log B + 1)\frac{n}{\log n} + C\frac{n(\log\log n)^2}{(\log n)^2}\right]\end{aligned} \tag{2.12}$$

for all $n \ge 3$.

Proof. Denote the integral on the left-hand side of (2.12) by I_n. It is convenient to rewrite this integral as

$$I_n = \int_0^\infty \exp(\psi_n(x))\, dx,$$

where we denote

$$\psi_n(x) = n \log x - Be^x. \tag{2.13}$$

To obtain an effective bound on this integral, it is natural to seek the point where $\psi_n(x)$ is maximized. Examining its derivative $\psi_n'(x) = n/x - Be^x$, we see that it is positive for x positive and close to 0, negative for large values of x, and crosses zero when

$$xe^x = n/B,$$

an equation that has a unique solution, which we denote x_n, that is expressible in terms of the Lambert W-function, namely as

$$x_n = W(n/B).$$

Thus x_n is the unique global maximum point of $\psi_n(x)$. By (2.11), the asymptotic behavior of x_n for large n (with B fixed) as $n \to \infty$ is given by

$$\begin{aligned} x_n &= \log\left(\frac{n}{B}\right) - \log\log\left(\frac{n}{B}\right) + \frac{\log\log\left(\frac{n}{B}\right)}{\log\left(\frac{n}{B}\right)} + O\left(\left(\frac{\log\log\left(\frac{n}{B}\right)}{\log\left(\frac{n}{B}\right)}\right)^2\right) \\ &= (\log n - \log B) - \left(\log\log n - \frac{\log B}{\log n} + O\left(\left(\frac{\log B}{\log n}\right)^2\right)\right) \\ &\quad + \frac{\log\log n - \frac{\log B}{\log n} + O\left(\left(\frac{\log B}{\log n}\right)^2\right)}{\log n - \log B} + O\left(\left(\frac{\log\log n}{\log n}\right)^2\right) \\ &= \log n - \log\log n - \log B + \frac{\log B}{\log n} \\ &\quad + \frac{\log\log n}{\log n} + O\left(\left(\frac{\log\log n}{\log n}\right)^2\right). \end{aligned} \tag{2.14}$$

Denote $A_n = \psi_n(x_n)$, and observe that we can use the defining relation $x_n e^{x_n} = n/B$ for x_n to rewrite A_n in the form

$$\begin{aligned} A_n &= n \log x_n - Be^{x_n} = n \log(x_n e^{x_n}) - n x_n - \frac{B}{x_n}(x_n e^{x_n}) \\ &= n \log\left(\frac{n}{B}\right) - n x_n - \frac{n}{x_n} = n\left(\log n - \log B - x_n - \frac{1}{x_n}\right). \end{aligned} \tag{2.15}$$

This form for A_n makes it straightforward to derive an asymptotic formula for A_n: first, estimate the term $1/x_n$ separately as

$$\begin{aligned}\frac{1}{x_n} &= \frac{1}{\log n - \log\log n - \log B + O\left(\frac{\log\log n}{\log n}\right)} \\ &= \frac{1}{\log n}\left(1 - \frac{\log\log n}{\log n} - \frac{\log B}{\log n} + O\left(\frac{\log\log n}{\log n}\right)\right)^{-1} \\ &= \frac{1}{\log n} + O\left(\frac{\log\log n}{(\log n)^2}\right).\end{aligned} \tag{2.16}$$

Then inserting (2.14) and (2.16) into (2.15) gives

$$\begin{aligned}A_n = n\log\log n &- \frac{n\log\log n}{\log n} \\ &- (\log B + 1)\frac{n}{\log n} + O\left(\frac{n(\log\log n)^2}{(\log n)^2}\right) \qquad (n\to\infty).\end{aligned} \tag{2.17}$$

We can now use these estimates to bound the integral I_n. First, split it into two parts, writing it as $I_n = I_n^{(1)} + I_n^{(2)}$, where

$$I_n^{(1)} = \int_0^{2\log n} \exp(\psi_n(x))\,dx, \qquad I_n^{(2)} = \int_{2\log n}^{\infty} \exp(\psi_n(x))\,dx.$$

Since $\psi_n(x) \le A_n$ for all $x > 0$, for the first integral we have the trivial bound

$$\begin{aligned}I_n^{(1)} &\le 2\log n \cdot e^{A_n} \\ &= \exp\left[n\log\log n - \frac{n\log\log n}{\log n} - (\log B + 1)\frac{n}{\log n} + O\left(\frac{n(\log\log n)^2}{(\log n)^2}\right)\right].\end{aligned} \tag{2.18}$$

To bound the second integral, observe that $\psi_n(x)$ is a concave function (since its second derivative is everywhere negative), so in particular it is bounded from above by its tangent line at $x = 2\log n$; that is, we have the inequality

$$\psi_n(x) \le \psi_n(2\log n) + \psi_n'(2\log n)(x - 2\log n) \qquad (x > 0).$$

The constants $\psi_n(2\log n)$, $\psi_n'(2\log n)$ in this inequality satisfy, for n large enough,

$$\begin{aligned}\psi_n(2\log n) &= n\log(2\log n) - Bn^2 \le -\frac{B}{2}n^2 \le -\frac{1}{2}n^2, \\ \psi_n'(2\log n) &= \frac{n}{2\log n} - Bn^2 \le -\frac{B}{2}n^2 \le -\frac{1}{2}n^2.\end{aligned}$$

This then implies that, again for large n, we have

$$
\begin{aligned}
(2.19)\qquad I_n^{(2)} &\le \int_{2\log n}^{\infty} \exp\big(\psi_n(2\log n) + \psi_n'(2\log n)(x - 2\log n)\big)\,dx \\
&= \exp(\psi_n(2\log n)) \int_0^{\infty} \exp(\psi_n'(2\log n)t)\,dt \\
&= \frac{1}{-\psi_n'(2\log n)} \exp(\psi_n(2\log n)) \le \frac{2}{n^2} e^{-n^2/2} = O(1).
\end{aligned}
$$

Combining (2.18) and (2.19) gives the claimed bound (2.12). ∎

We are ready to prove (2.3). First, consider the following slightly informal calculation that essentially explains how the expansion (2.2) arises out of the definition (2.1) of the coefficients b_n. Invoking the formula (A.5) for the generating function for the Hermite polynomials, we have

$$
\begin{aligned}
(2.20)\qquad &\sum_{n=0}^{\infty} (-1)^n b_{2n} H_{2n}(t) \\
&= \sum_{n=0}^{\infty} i^n b_n H_n(t) = \sum_{n=0}^{\infty} \frac{i^n}{2^n n!} \int_{-\infty}^{\infty} x^n e^{-x^2/4} \varPhi(x)\,dx \cdot H_n(t) \\
&= \int_{-\infty}^{\infty} \bigg(\sum_{n=0}^{\infty} \frac{i^n}{2^n n!} x^n H_n(t) \bigg) e^{-x^2/4} \varPhi(x)\,dx \\
&= \int_{-\infty}^{\infty} \exp\bigg(2t \cdot \frac{ix}{2} - \Big(\frac{ix}{2}\Big)^2 \bigg) e^{-x^2/4} \varPhi(x)\,dx = \int_{-\infty}^{\infty} e^{itx} \varPhi(x)\,dx = \varXi(t),
\end{aligned}
$$

which is (2.2). Note that at the heart of this calculation is the simple identity

$$
(2.21)\qquad e^{itx} = e^{-x^2/4} \sum_{n=0}^{\infty} \frac{i^n x^n}{2^n n!} H_n(t),
$$

a trivial consequence of (A.5), which expands the Fourier transform integration kernel e^{itx} as an infinite series in the Hermite polynomials. Thus, to get the more precise statement (2.3), all that is left to do is to perform the same calculation a bit more carefully, using the results of Lemmas 2.4 and 2.6 to get more explicit error bounds when summing this infinite series and integrating. Namely, using (2.21) we can estimate the left-hand side of (2.3) as

$$
\begin{aligned}
(2.22)\qquad \Big| \varXi(t) - \sum_{n=0}^{N} (-1)^n b_{2n} H_{2n}(t) \Big| &= \Big| \varXi(t) - \sum_{n=0}^{2N} i^n b_n H_n(t) \Big| \\
&= \bigg| \int_{-\infty}^{\infty} \varPhi(x) \bigg(e^{itx} - e^{-x^2/4} \sum_{n=0}^{2N} \frac{i^n x^n}{2^n n!} H_n(t) \bigg)\,dx \bigg|
\end{aligned}
$$

$$
\begin{aligned}
&= \left| \int_{-\infty}^{\infty} \Phi(x) e^{-x^2/4} \sum_{n=2N+1}^{\infty} \frac{i^n x^n}{2^n n!} H_n(t)\, dx \right| \\
&\le \sum_{n=2N+1}^{\infty} \frac{1}{2^n n!} \Big(\int_{-\infty}^{\infty} \Phi(x) e^{-x^2/4} |x|^n \, dx \Big) |H_n(t)| \\
&= \sum_{n=2N+1}^{\infty} \frac{1}{2^{n-1} n!} \Big(\int_{0}^{\infty} \Phi(x) e^{-x^2/4} x^n \, dx \Big) |H_n(t)| \\
&\le \sum_{n=2N+1}^{\infty} \frac{1}{2^{n-1} n!} C \exp\Big(\frac{3}{4} n \log n \Big) \int_{0}^{\infty} \Phi(x) e^{-x^2/4} x^n \, dx
\end{aligned}
$$

for all t ranging over some fixed compact set $K \subset \mathbb{C}$, and where in the last step we appealed to Lemma 2.4, with C denoting the positive constant given by that lemma (depending on K).

Now, since $\Phi(x) = O(\exp(-3e^{2x}))$ as $x \to \infty$ by (2.8), we can use Lemma 2.6 with $B = 3$ to bound the integral in the last sum in (2.22), and therefore conclude that this sum is bounded from above by

$$
C \sum_{n=2N+1}^{\infty} \frac{1}{2^n n!} \exp\Big(\frac{3}{4} n \log n \Big) \times \frac{1}{2^n} \exp\Big(n \log\log n - \frac{n \log\log n}{\log n} + O\Big(\frac{n}{\log n} \Big) \Big).
$$

By Stirling's formula this is $O\big(\exp\big(-\frac{1}{5} N \log N\big)\big)$, which is the bound we need. The proof of Theorem 2.1 is complete. ∎

Proof of Corollary 2.2. The Hermite polynomials form an orthogonal basis of the Hilbert space $L^2(\mathbb{R}, e^{-t^2} dt)$. By Lemma 2.6 we also get an upper bound for the coefficients b_{2n} (which will be superseded by a more precise asymptotic result in the next section, but is still useful), namely the statement that

$$
b_{2n} \le \frac{C}{2^{2n} (2n)!} \exp(2n \log\log(2n))
$$

for some constant $C > 0$ and all $n \ge 3$. Together with the fact that the squared L^2-norm of $H_n(t)$ is $\sqrt{\pi}\, 2^n n!$ (see (A.2)), this implies that the infinite series on the right-hand side of (2.2) converges in the sense of the function space $L^2(\mathbb{R}, e^{-t^2} dt)$ to an element of this space. Since L^2-convergence implies almost everywhere convergence along a subsequence, the L^2-limit must be equal to the pointwise limit, that is, the function $\Xi(t)$. Thus, the relation (2.2) holds in the sense of L^2, and it follows that the coefficients in the expansion can be extracted in the standard way as inner products in the L^2-space, which (again because of (A.2)) leads to the formula (2.4). ∎

2.4. An asymptotic formula for the coefficients b_{2n}. We now refine our analysis of the Hermite expansion by deriving an asymptotic formula for the coefficients b_{2n}. These asymptotics are most simply expressed in terms of the Lambert W-function.

THEOREM 2.7 (Asymptotic formula for the coefficients b_{2n}). *The coefficients b_{2n} satisfy the asymptotic formula*

$$b_{2n} = \left(1 + O\left(\frac{\log\log n}{\log n}\right)\right) \frac{\pi^{1/4}}{2^{4n-5/2}(2n)!} \left(\frac{2n}{\log(2n)}\right)^{7/4} \times \exp\left[2n\left(\log\left(\frac{2n}{\pi}\right) - W\left(\frac{2n}{\pi}\right) - \frac{1}{W\left(\frac{2n}{\pi}\right)}\right) - \frac{1}{16} W\left(\frac{2n}{\pi}\right)^2\right] \tag{2.23}$$

as $n \to \infty$.

The appearance of the non-elementary, implicitly defined function $W(x)$ in (2.23) may make it somewhat difficult to use or to gain intuition from, but with the help of the asymptotic formula (2.11) for the Lambert W-function, or its stronger version [15, eq. (4.19)] mentioned above, we can extract the asymptotically dominant terms from inside the exponential to get an asymptotic formula involving more familiar functions (unfortunately, at a cost of having a much larger error term—but this seems like an unavoidable tradeoff that comes about as a result of the unusual asymptotic expansion of the Lambert W-function). For example, as an immediate corollary we get the following more explicit, but weaker, result.

COROLLARY 2.8 (Asymptotic formula for the logarithm of the coefficients b_{2n}). *We have the relation*

$$\log b_{2n} = -2n\log(2n) + 2n\log\log\frac{2n}{\pi} + O(n) \tag{2.24}$$

as $n \to \infty$.

Proof of Theorem 2.7. Define numbers Q_n, r_n by

$$Q_n = \int_0^\infty x^{2n} e^{-x^2/4} e^{5x/2} \left(e^{2x} - \frac{3}{2\pi}\right) \exp(-\pi e^{2x})\, dx, \tag{2.25}$$

$$r_n = \int_0^\infty x^{2n} e^{-x^2/4} e^{5x/2} \sum_{m=2}^\infty \left(m^4 e^{2x} - \frac{3m^2}{2\pi}\right) \exp(-\pi m^2 e^{2x})\, dx, \tag{2.26}$$

so that, by (1.8) and (2.1),

$$b_{2n} = \frac{\pi^2}{2^{2n-3}(2n)!}(Q_n + r_n). \tag{2.27}$$

We will analyze the asymptotic behavior of Q_n and then show that the contribution of r_n is asymptotically negligible relative to that of Q_n.

Part 1: *Analysis of Q_n using Laplace's method.* Define a function

$$f(x) = e^{-x^2/4} e^{5x/2}\left(e^{2x} - \frac{3}{2\pi}\right).$$

Then Q_n can be rewritten in the form

$$Q_n = \frac{1}{2^{2n}} \int_0^\infty f(x)\exp(\psi_{2n}(2x))\,dx, \tag{2.28}$$

where $\psi_{2n}(x)$ is defined in (2.13), with the specific parameter value $B = \pi$. This representation makes it possible to use Laplace's method to understand the asymptotic behavior of Q_n as n grows large. Proceeding as in the proof of Lemma 2.6, we recall our observation that the function $\psi_{2n}(x)$ has a unique global maximum point at

$$x_{2n} = W\left(\frac{2n}{\pi}\right).$$

Now let quantities $\alpha_n, \beta_n, \gamma_n$ be defined by

$$\alpha_n = \psi_{2n}(x_{2n}), \tag{2.29}$$

$$\beta_n = -\psi''_{2n}(x_{2n}), \tag{2.30}$$

$$\gamma_n = f(x_{2n}/2). \tag{2.31}$$

Examining these quantities a bit more closely, note that $\alpha_n = A_{2n}$ in the notation used in the proof of Lemma 2.6 (again with the parameter $B = \pi$), so that, as in (2.15), we have

$$\alpha_n = 2n\left(\log(2n) - \log\pi - x_{2n} - \frac{1}{x_{2n}}\right). \tag{2.32}$$

For β_n we have

$$\beta_n = \frac{2n}{x_{2n}^2} + \pi e^{x_{2n}} = \frac{2n}{x_{2n}^2} + \frac{2n}{x_{2n}} = \left(1 + O\left(\frac{1}{\log n}\right)\right)\frac{2n}{x_{2n}}, \tag{2.33}$$

and for γ_n we can write

$$\begin{aligned} \gamma_n &= (1 + O(e^{-x_{2n}}))\exp\left(-\frac{1}{16}x_{2n}^2 + \frac{9}{4}x_{2n}\right) \\ &= \left(1 + O\left(\frac{\log n}{n}\right)\right)\left(\frac{2n}{\pi x_{2n}}\right)^{9/4}\exp\left(-\frac{1}{16}x_{2n}^2\right). \end{aligned} \tag{2.34}$$

With these preparations, Laplace's method in its heuristic form predicts that the integral on the right-hand side of (2.28) is given approximately for large n by the expression

$$\frac{\sqrt{\pi}}{\sqrt{-2\psi''_{2n}(x_{2n})}} f(x_{2n}/2)\exp(\psi_{2n}(x_n)) = \frac{\sqrt{\pi}}{\sqrt{2\beta_n}}\gamma_n \exp(\alpha_n). \tag{2.35}$$

Our goal is to establish this rigorously, with a precise rate of convergence estimate; substituting (2.32)–(2.34) into (2.35) will then give the desired formula for Q_n.

It will be convenient to split up the integral defining Q_n into three parts and estimate each part separately. Denote $\mu_n = n^{-2/5}$, and denote by J_n the interval $\left[\frac{1}{2}x_{2n} - \mu_n, \frac{1}{2}x_{2n} + \mu_n\right]$. Now let

$$Q_n^{(1)} = \int_0^{\frac{1}{2}x_{2n}-\mu_n} f(x)\exp(\psi_{2n}(2x))\,dx, \qquad Q_n^{(2)} = \int_{J_n} f(x)\exp(\psi_{2n}(2x))\,dx,$$

$$Q_n^{(3)} = \int_{\frac{1}{2}x_{2n}+\mu_n}^{\infty} f(x)\exp(\psi_{2n}(2x))\,dx,$$

so that $Q_n = \frac{1}{2^{2n}}(Q_n^{(1)} + Q_n^{(2)} + Q_n^{(3)})$. Our estimates will rely on the following useful calculus observations (the first two of which were already noted in the proof of Lemma 2.6):

(1) The function $\psi_{2n}(x)$ is increasing on $(0, x_{2n})$ and decreasing on (x_{2n}, ∞).
(2) The function $\psi_{2n}(x)$ is concave.
(3) $\sup_{x\in J_n} |\psi_{2n}'''(2x)| = O(n)$ as $n \to \infty$. Indeed, $\psi_{2n}'''(2x) = \frac{n}{2x^3} - \pi e^{2x}$, so, for $x \in J_n$, using the fact that (by (2.14)) for n large enough we have the relation $J_n \subseteq \left[\frac{1}{4}\log n, \frac{1}{2}\log n\right]$, we get

$$|\psi_{2n}'''(2x)| \le \frac{n}{2x^3} + \pi e^{2x} \le \frac{4^3 n}{2\log^3 n} + \pi e^{\log n} = O(n).$$

(4) As a consequence of the last observation, the Taylor expansion of $\psi_{2n}(2x)$ around $x = \frac{1}{2}x_{2n}$ in the interval J_n has the form

$$\psi_{2n}(2x) = \alpha_n - 2\beta_n\left(x - \frac{x_{2n}}{2}\right)^2 + O\left(n\left|x - \frac{x_{2n}}{2}\right|^3\right) \qquad (x \in J_n), \tag{2.36}$$

where the constant implicit in the big-O term does not depend on n or x.
(5) $\sup_{x\in J_n}\left|\frac{f(x)}{f(x_{2n}/2)} - 1\right| = O\left(\frac{\log n}{n^{2/5}}\right)$. Indeed, noting that $x_n \to \infty$ as $n \to \infty$, so that $f(x_{2n}/2) \ge \frac{1}{2}e^{-x_{2n}^2/16 + 9x_{2n}/4}$ if n is large, we have

$$\left|\frac{f(x)}{f(x_{2n}/2)} - 1\right| = \left|\frac{e^{-\frac{x^2}{4}+\frac{9}{2}x} - \frac{3}{2\pi}e^{-\frac{x^2}{4}+\frac{5}{2}x}}{e^{-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}} - \frac{3}{2\pi}e^{-\frac{x_{2n}^2}{16}+\frac{5}{4}x_{2n}}} - 1\right| \tag{2.37}$$

$$= \left|\frac{\left(e^{-\frac{x^2}{4}+\frac{9}{2}x} - \frac{3}{2\pi}e^{-\frac{x^2}{4}+\frac{5}{2}x}\right) - \left(e^{-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}} - \frac{3}{2\pi}e^{-\frac{x_{2n}^2}{16}+\frac{5}{4}x_{2n}}\right)}{e^{-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}} - \frac{3}{2\pi}e^{-\frac{x_{2n}^2}{16}+\frac{5}{4}x_{2n}}}\right|$$

$$\leq \left| \frac{e^{-\frac{x^2}{4}+\frac{9}{2}x} - e^{-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}}}{\frac{1}{2}e^{-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}}} \right| + \frac{3}{2\pi}\left| \frac{e^{-\frac{x^2}{4}+\frac{5}{2}x} - e^{-\frac{x_{2n}^2}{16}+\frac{5}{4}x_{2n}}}{\frac{1}{2}e^{-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}}} \right|$$

$$= 2\left|e^{\left(-\frac{x^2}{4}+\frac{9}{2}x\right)-\left(-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}\right)} - 1\right|$$

$$+ \frac{6}{2\pi}e^{-x_{2n}}\left|e^{\left(-\frac{x^2}{4}+\frac{5}{2}x\right)-\left(-\frac{x_{2n}^2}{16}+\frac{5}{4}x_{2n}\right)} - 1\right|.$$

Now observe that $e^{-x_{2n}} = O(1)$, and that for $x \in J_n$ we have

$$\left|\left(-\frac{x^2}{4}+\frac{9}{2}x\right) - \left(-\frac{x_{2n}^2}{16}+\frac{9}{4}x_{2n}\right)\right|$$
$$\leq \frac{9}{2}\left|x - \frac{x_{2n}}{2}\right| + \frac{1}{4}\left|x - \frac{x_{2n}}{2}\right| \cdot \left|x + \frac{x_{2n}}{2}\right| = O\left(\frac{\log n}{n^{2/5}}\right)$$

(with a uniform constant implicit in the big-O term), and similarly

$$\left|\left(-\frac{x^2}{4}+\frac{5}{2}x\right) - \left(-\frac{x_{2n}^2}{16}+\frac{5}{4}x_{2n}\right)\right| = O\left(\frac{\log n}{n^{2/5}}\right),$$

so that (2.37) implies the claimed bound.

We are ready to evaluate the integrals $Q_n^{(1)}$, $Q_n^{(2)}$, $Q_n^{(3)}$, starting with the middle integral $Q_n^{(2)}$, which is the one that is the most significant asymptotically. The standard idea is that the exponential term $\exp(\psi_{2n}(2x))$ can be approximated by a Gaussian centered around the point $\frac{1}{2}x_{2n}$. This follows from the Taylor expansion (2.36). Indeed, making the change of variables $u = \sqrt{\beta_n}\left(x - \frac{1}{2}x_{2n}\right)$ in the integral, we have

$$(2.38)\qquad Q_n^{(2)} = \int_{J_n} f(x)\exp(\psi_{2n}(2x))\,dx$$

$$= \int_{-\mu_n\sqrt{\beta_n}}^{\mu_n\sqrt{\beta_n}} f\left(\frac{x_{2n}}{2} + \frac{u}{\sqrt{\beta_n}}\right)\exp\left(\psi_{2n}\left(x_{2n} + \frac{2u}{\sqrt{\beta_n}}\right)\right)\frac{du}{\sqrt{\beta_n}}$$

$$= \frac{1}{\sqrt{\beta_n}}\int_{-\mu_n\sqrt{\beta_n}}^{\mu_n\sqrt{\beta_n}}\left(1 + O\left(\frac{\log n}{n^{2/5}}\right)\right) f\left(\frac{x_{2n}}{2}\right)\exp\left[\alpha_n - 2u^2 + O\left(n\frac{|u|^3}{\beta_n^{3/2}}\right)\right] du$$

$$= \left(1 + O\left(\frac{\log n}{n^{2/5}}\right)\right)\left(1 + O\left(\frac{1}{n^{1/5}}\right)\right)\frac{1}{\sqrt{\beta_n}}e^{\alpha_n}\gamma_n\int_{-\mu_n\sqrt{\beta_n}}^{\mu_n\sqrt{\beta_n}} e^{-2u^2}\,du$$

$$= \left(1 + O\left(\frac{1}{n^{1/5}}\right)\right)\frac{1}{\sqrt{\beta_n}}\gamma_n e^{\alpha_n}\left[\sqrt{\frac{\pi}{2}} - O\left(\frac{1}{\mu_n\sqrt{\beta_n}}\exp(-2\mu_n^2\beta_n)\right)\right]$$

$$= \left(1 + O\left(\frac{1}{n^{1/5}}\right)\right)\frac{\sqrt{\pi}}{\sqrt{2\beta_n}}\gamma_n e^{\alpha_n},$$

where in the penultimate step we used the standard inequality

$$\int_t^\infty e^{-u^2/2}\,du \le \frac{1}{t}e^{-t^2/2} \qquad (t>0). \tag{2.39}$$

Next, to estimate $Q_n^{(1)}$, we use the fact that $\psi_{2n}(2x)$ is increasing on the interval of integration, bounding the integral by the length of the integration interval multiplied by an upper bound for $f(x)$ and the value of $\exp(\psi_{2n}(2x))$ at the rightmost end of the interval. Note that $f(x)$ is bounded from above by the numerical constant

$$K_0 := \left(\sup_{x\ge 0} e^{-x^2/4+9x/2} + \frac{3}{2\pi}\sup_{x\ge 0} e^{-x^2/4+5x/2}\right) = e^{81/4} + \frac{3}{2\pi}e^{25/4}.$$

Thus, using (2.33), (2.34) and (2.36), we get

$$\begin{aligned} Q_n^{(1)} &\le K_0\left(\frac{x_{2n}}{2} - \mu_n\right)\exp(\psi_{2n}(x_{2n}-2\mu_n)) \\ &\le \frac{K_0}{2}x_{2n}\exp(\alpha_n - 2\beta_n\mu_n^2 + O(n\mu_n^3)) \\ &= O(\log n)e^{\alpha_n}O(\exp(-n^{1/10}))\left(1+O\left(\frac{1}{n^{1/5}}\right)\right) \\ &= O\left(e^{-\frac{1}{2}n^{1/10}}\frac{\sqrt{\pi}}{\sqrt{2\beta_n}}\gamma_n e^{\alpha_n}\right). \end{aligned} \tag{2.40}$$

Next, to estimate $Q_n^{(3)}$, note that, as in the proof of Lemma 2.6, by the concavity of $\psi_{2n}(2x)$ the graph of $\psi_{2n}(2x)$ is bounded from above by the tangent line to the graph at $x = x_{2n}/2+\mu_n$. In other words, we have

$$\psi_{2n}(2x) \le \psi_{2n}(x_{2n}+2\mu_n) + 2\psi_{2n}'(x_{2n}+2\mu_n)\left(x - \frac{x_{2n}}{2} - \mu_n\right) \qquad (x>0).$$

Moreover, it is useful to note that the derivative value $\psi_{2n}'(x_{2n}+2\mu_n)$ satisfies

$$\begin{aligned} \psi_{2n}'(x_{2n}+2\mu_n) &= \frac{2n}{x_{2n}+2\mu_n} - \pi e^{x_{2n}+2\mu_n} = \frac{2n}{x_{2n}+2\mu_n} - e^{2\mu_n}\frac{2n}{x_{2n}} \\ &\le \frac{2n}{x_{2n}}(1-e^{2\mu_n}) \le -\frac{4n\mu_n}{x_{2n}}, \end{aligned}$$

so in particular $\psi_{2n}'(x_{2n}+2\mu_n) \le -1$ if n is large enough. These observations imply that as $n\to\infty$, $Q_n^{(3)}$ satisfies the bound

$$\begin{aligned} Q_n^{(3)} \le K_0 \int_{\frac{1}{2}x_{2n}+\mu_n}^\infty \exp\Bigg(&\psi_{2n}(x_{2n}+2\mu_n) \\ &+ 2\psi_{2n}'(x_{2n}+2\mu_n)\left(x - \frac{x_{2n}}{2} - \mu_n\right)\Bigg)\,dx \end{aligned} \tag{2.41}$$

$$\leq K_0 \int_{\frac{1}{2}x_{2n}+\mu_n}^{\infty} \exp(\alpha_n - 2\beta_n\mu_n^2 + O(n\mu_n^3)) \exp\left(-\left(x - \frac{x_{2n}}{2} - \mu_n\right)\right) dx$$

$$= K_0\left(1 + O\left(\frac{1}{n^{1/5}}\right)\right) e^{\alpha_n} O(\exp(-n^{1/10})) \int_0^{\infty} \exp(-u)\, du$$

$$= O\left(e^{-n^{1/10}} \frac{\sqrt{\pi}}{\sqrt{2\beta_n}} \gamma_n e^{\alpha_n}\right).$$

Combining (2.38), (2.40) and (2.41), we finally have

$$Q_n = \left(1 + O\left(\frac{1}{n^{1/5}}\right)\right) \frac{\sqrt{\pi}}{2^{2n}\sqrt{2\beta_n}} \gamma_n e^{\alpha_n}. \tag{2.42}$$

Using (2.32)–(2.34) we now get the asymptotic formula

$$Q_n = \left(1 + O\left(\frac{1}{\log n}\right)\right) \frac{1}{2^{2n+1/2}} \left(\frac{2n}{\pi x_{2n}}\right)^{7/4} \times \exp\left[2n\left(\log(2n) - \log\pi - x_{2n} - \frac{1}{x_{2n}}\right) - \frac{1}{16}x_{2n}^2\right] \tag{2.43}$$

as $n \to \infty$. In particular, for the purpose of comparing Q_n to r_n, it is useful to note that the exponential factors $1/2^{2n}$ and e^{α_n} are asymptotically the most significant ones in (2.42). More precisely, recalling (2.14), (2.17), (2.33) and (2.34), we get that

$$\begin{aligned} Q_n &= \frac{1}{2^{2n}} \exp\big(\alpha_n + O((\log n)^2)\big) \\ &= \frac{1}{2^{2n}} \exp\bigg[2n\log\log(2n) - \frac{2n\log\log(2n)}{\log(2n)} \\ &\qquad - (\log\pi + 1)\frac{2n}{\log(2n)} + O\left(\frac{n(\log\log n)^2}{(\log n)^2}\right)\bigg] \quad \text{as } n \to \infty. \end{aligned} \tag{2.44}$$

Part 2: *Estimating* r_n. We proceed with asymptotically bounding r_n. Observe that, by (2.9), r_n satisfies

$$|r_n| \leq C_1 \int_0^{\infty} x^{2n} \exp(-3\pi e^{2x})\, dx = \frac{C_1}{2^{2n+1}} \int_0^{\infty} u^{2n} \exp(-3\pi e^u)\, du$$

for some constant $C_1 > 0$. We can therefore once again apply Lemma 2.6, this time with the parameter $B = 3\pi$, to deduce that, for all $n \geq 3$ and some constant $C_2 > 0$,

$$|r_n| \leq \frac{1}{2^{2n}} \exp\bigg[2n\log\log(2n) - \frac{2n\log\log(2n)}{\log(2n)} - (\log(3\pi) + 1)\frac{2n}{\log(2n)} + C_2 \frac{2n(\log\log(2n))^2}{(\log(2n))^2}\bigg].$$

Comparing this to (2.44), we see that, for large n,

$$|r_n| \le \exp\left(-\frac{1}{2}\log(3)\frac{2n}{\log(2n)}\right)Q_n. \tag{2.45}$$

Thus r_n is indeed asymptotically negligible compared to Q_n.

PART 3: *Finishing the proof.* Combining (2.27), (2.43) and (2.45) we finally arrive at the desired formula for b_{2n}:

$$\begin{aligned} b_{2n} &= \frac{\pi^2}{2^{2n-3}(2n)!}\left(1+O\left(\exp\left(-\log(3)\frac{n}{\log(2n)}\right)\right)\right)Q_n \\ &= \left(1+O\left(\frac{1}{\log n}\right)\right)\frac{\pi^2}{2^{2n-3}(2n)!}\times\frac{1}{2^{2n+1/2}}\left(\frac{2n}{\pi x_{2n}}\right)^{7/4} \\ &\quad\times\exp\left[2n\left(\log(2n)-\log\pi - x_{2n}-\frac{1}{x_{2n}}\right)-\frac{1}{16}x_{2n}^2\right]. \end{aligned}$$

Since $x_{2n} = W\big(\frac{2n}{\pi}\big) = \big(1+O\big(\frac{\log\log n}{\log n}\big)\big)\log(2n)$, this gives (2.23) and completes the proof of Theorem 2.7. ∎

2.5. The Poisson flow, Pólya–de Bruijn flow and de Bruijn–Newman constant. One recurring theme in the study of the Riemann Hypothesis is the idea that in order to understand the zeros of the Riemann xi (or zeta) function, one might start by looking at suitable approximations to it that have a simpler structure—for example, being polynomials instead of entire or meromorphic functions—and trying to understand the location of the zeros of those approximations first. The hope is that there exists some good approximation that would have the feature that the zeros of the approximating functions can be understood, and, in an ideal scenario, shown to all lie on the real line (or on the critical line $\mathrm{Re}(s) = 1/2$, depending on the coordinate system used). In the setting of a discrete sequence of approximations, this approach has been applied for example to the partial sums of the Taylor series of $\Xi(t)$ (see [30]) and to the partial sums of the Dirichlet series of $\zeta(s)$ (see [23, 62, 65]). While those attacks can involve the use of some rather ingenious and sophisticated tools, they have not resulted in any easily quantifiable progress on the original question of RH.

Instead of looking at a discrete sequence of approximations, certain other contexts naturally suggest instead a family of approximations indexed by a continuous parameter. We refer to such a family informally, especially in the case when the family satisfies a partial differential equation or some other sort of dynamical evolution law (all the approximation families we consider will be of this type), as a *flow*.

One very natural and well-studied example of such a flow is the family of functions

$$\Xi_\lambda(t) = \int_{-\infty}^{\infty} e^{\lambda x^2} \Phi(x) e^{itx}\, dx \qquad (\lambda \in \mathbb{R}). \tag{2.46}$$

For $\lambda = 0$, we have $\Xi_0 \equiv \Xi$, so the family Ξ_λ is a flow passing through the Riemann xi function at $\lambda = 0$. We refer to it as the *Pólya–de Bruijn flow* associated with the xi function; this term seems appropriate in view of Pólya's discovery of universal factors described in Section 1.1 and its extension by de Bruijn. Specifically, Pólya's result described in the Introduction to the effect that $e^{\lambda x^2}$ is a universal factor implies that the Pólya–de Bruijn flow preserves *hyperbolicity* (the property of an entire function of having no non-real zeros) in the positive direction of the "time" parameter λ: that is, if Ξ_λ is hyperbolic for some specific value of λ, then so is Ξ_μ for any $\mu > \lambda$, and in particular, if it could be shown that Ξ_λ is hyperbolic for some *negative* value $\lambda < 0$, the Riemann Hypothesis would follow. Moreover, showing that Ξ_λ is hyperbolic for *positive* values of λ (which by the same logic ought to be both more likely to be true, and easier to prove if true) may still be beneficial, since if for instance it could somehow be shown that Ξ_λ were hyperbolic for *all* $\lambda > 0$, once again RH would follow by a straightforward approximation argument.

De Bruijn extended Pólya's work in an important way when he showed that in fact Ξ_λ is hyperbolic for all $\lambda \geq 1/8$. His result was later strengthened slightly by Ki, Kim and Lee [31], who showed that the same would be true for $\lambda \geq 1/8 - \epsilon$ for some (fixed, but non-explicit) $\epsilon > 0$. In the negative direction, Newman [38] proved that Ξ_λ is *not* hyperbolic if λ is a negative number of sufficiently large magnitude, and conjectured that the same statement holds true for *all* $\lambda < 0$—this is usually formulated as the statement that the *de Bruijn–Newman constant*, denoted by Λ and defined as four times the greatest lower bound of the set of λ's for which Ξ_λ is hyperbolic ([2]), is non-negative. An explicit numerical lower bound of -50 for the de Bruijn–Newman constant was later established by Csordas, Norfolk and Varga [17]. The lower bound was pushed upwards further in a succession of papers [18, 19, 20, 40, 41, 60, 58], with the bounds established gradually growing extremely close to 0 on the negative side. Most recently Rodgers and Tao [59] succeeded in proving Newman's conjecture that $\Lambda \geq 0$, and recent work by the Polymath15 project [54] strengthened the result of Ki, Kim and Lee mentioned above by proving the sharper upper bound $\Lambda \leq 0.22$.

([2]) The multiplication by four is a quirk associated with the different notational conventions used by different authors. See [9, p. 63 and Table 5.2 on p. 68] for further discussion and a comparison of the different conventions.

We now come to a key idea that relates the above discussion to our theme of expansions of the Riemann xi function in families of orthogonal polynomials, and the Hermite polynomials in particular. Specifically, it is the idea that any series expansion of the Riemann xi function in a system of orthogonal polynomials comes equipped with its own flow based on the standard construction of the so-called *Poisson kernel* in the theory of orthogonal polynomials. We call this the *Poisson flow*.

To define the Poisson flow, recall that the Poisson kernel for a family $\phi = (\phi_n)_{n=0}^\infty$ of polynomials that are orthogonal with respect to a weight function $w(x)$ is defined by

$$p_r^\phi(x,y) = \sum_{n=0}^\infty \frac{r^n}{\int_{\mathbb{R}} \phi_n(u)^2 w(u)\,du} \phi_n(x)\phi_n(y) \qquad (|r|<1). \tag{2.47}$$

Its essential feature is the equation

$$\int_{-\infty}^{\infty} p_r^\phi(x,y)\phi_n(y)w(y)\,dy = r^n\phi_n(x),$$

which is trivial to verify by evaluating the integral termwise. That is, the associated integral kernel operator $\Pi_r^\phi : f \mapsto \int_{\mathbb{R}} p_r^\phi(x,y)f(y)w(y)\,dy$ acting on $L^2(\mathbb{R}, w(x)dx)$ sends a function with Fourier expansion $f(x) = \sum_n \gamma_n\phi_n$ to $\sum_n \gamma_n r^n \phi_n$, with the nth "harmonic" in the expansion being attenuated by a factor r^n. Note that one can also consider the limiting case $r \to 1$, in which case the definition (2.47) of the Poisson kernel p_r^ϕ no longer makes sense, but the operator Π_1^ϕ can be defined simply as the identity operator, which is clearly the limit of the Π_r's (and $p_1^\phi(x,y)$ can be thought of as the distribution $\delta(x-y)$).

We can now define the *Poisson flow associated with the Riemann xi function for the orthogonal polynomial sequence* $\phi = (\phi_n)$ to be the family of functions

$$\begin{aligned} X_r^\phi(t) &= \Pi_r^\phi(\Xi)(t) \\ &= \begin{cases} \int_{-\infty}^\infty p_r(t,\tau)\Xi(\tau)w(\tau)\,d\tau & \text{if } 0<r<1, \\ \Xi(t) & \text{if } r=1 \end{cases} \qquad (0<r\le 1). \end{aligned} \tag{2.48}$$

Alternatively, if $\Xi(t)$ is expressed in terms of its Fourier series expansion $\Xi(t) = \sum_{n=0}^\infty \gamma_n\phi_n(t)$ in the orthogonal polynomial family $(\phi_n)_{n=0}^\infty$ (in the sense of the function space $L^2(\mathbb{R}, w(x)dx)$), we can write the Poisson flow equivalently as

$$X_r^\phi(t) = \sum_{n=0}^\infty r^n\gamma_n\phi_n(t). \tag{2.49}$$

Denote the family of Hermite polynomials by $\mathcal{H} = (H_n)_{n=0}^\infty$, so that $p_r^{\mathcal{H}}(x,y)$ and $\Pi_r^{\mathcal{H}}$ now denote the Poisson kernel and integral operator associated with the Hermite polynomials, respectively, and $X_r^{\mathcal{H}}(t)$ denotes the corresponding flow associated with the Riemann xi function. Our main result for this section, relating the different concepts we introduced above, is the following.

THEOREM 2.9 (Connection between the Pólya–de Bruijn and Poisson flows). *The Poisson flow for the Hermite polynomials is related to the Pólya–de Bruijn flow* (2.46) *via*

$$X_r^{\mathcal{H}}(t) = \Xi_{(r^2-1)/4}(rt) \qquad (0 < r \le 1). \tag{2.50}$$

Proof. This is a straightforward calculation that generalizes (2.20) by weighting each of the summands in the expansion by the factor r^n. Once again using the generating function formula (A.5), we have

$$\begin{aligned} X_r^{\mathcal{H}}(t) &= \sum_{n=0}^\infty i^n r^n b_n H_n(t) = \sum_{n=0}^\infty \frac{i^n r^n}{2^n n!} \int_{-\infty}^\infty x^n e^{-x^2/4} \Phi(x)\, dx \cdot H_n(t) \\ &= \int_{-\infty}^\infty \bigg(\sum_{n=0}^\infty \frac{1}{n!} \Big(\frac{irx}{2}\Big)^n H_n(t) \bigg) e^{-x^2/4} \Phi(x)\, dx \\ &= \int_{-\infty}^\infty \exp\bigg(2t \cdot \frac{irx}{2} - \Big(\frac{irx}{2}\Big)^2 \bigg) e^{-x^2/4} \Phi(x)\, dx \\ &= \int_{-\infty}^\infty \Phi(x) \exp\bigg((r^2-1)\frac{x^2}{4} \bigg) e^{irtx}\, dx = \Xi_{(r^2-1)/4}(rt), \end{aligned} \tag{2.51}$$

as claimed. ∎

Theorem 2.9 ties together in an interesting way the different threads of research into RH begun with the work of Pólya on universal factors (and continued with the extensive subsequent investigations into the de Bruijn–Newman constant by de Bruijn, Newman and others) on the one hand, and Turán's ideas on the Hermite expansion on the other hand. Incidentally, hints of this connection seem to have already been noted in a less explicit way in the literature; see in particular [8, Section 3].

One key point to take away from this discussion is that the Poisson flow appears to be a natural device with which to try to approximate the Riemann xi function. And while Theorem 2.9 shows that the Poisson flow associated with the Hermite polynomials is equivalent to an already well-studied construction, the point is that Poisson flows are a method of approximation that allows us a considerable freedom in choosing the system of orthogonal polynomials to use, and it is conceivable that this might lead to new families of approximations with useful properties. Indeed, in Section 3, when we consider the expansion of $\Xi(t)$ in the family of Meixner–Pollaczek orthogonal polynomials f_n, we will revisit the Poisson flow in the context of this new expansion and show that it has some quite natural and interesting properties in that setting.

As a final remark, we recall that one of several notable features of the Pólya–de Bruijn flow, first pointed out in [20], is that it satisfies the time-reversed heat equation

$$\frac{\partial \Xi_\lambda(t)}{\partial \lambda} = -\frac{\partial^2 \Xi_\lambda(t)}{\partial t^2}, \tag{2.52}$$

a fact that follows immediately from the representation (2.46) by differentiating under the integral sign, and which played a useful role in the study of the de Bruijn–Newman constant (see [9, Sec. 5.5], [20], [59]). It is of some interest to note that the same result can also be obtained by using the relation (2.50) interpreting the Pólya–de Bruijn flow as a reparametrized version of the Poisson flow, together with basic properties of the Hermite polynomials. To see this, start by inverting (2.50) to express $\Xi_\lambda(t)$ in terms of the Poisson flow as

$$\Xi_\lambda(t) = X^{\mathcal{H}}_{\sqrt{1+4\lambda}}\left(\frac{t}{\sqrt{1+4\lambda}}\right).$$

Now expanding the Poisson flow as in (2.49), we differentiate and then use the classical ordinary differential equation (A.4) satisfied by the Hermite polynomials, to get

$$\begin{aligned}
\frac{\partial \Xi_\lambda(t)}{\partial \lambda} &= \frac{\partial}{\partial \lambda}\left(X^{\mathcal{H}}_{\sqrt{1+4\lambda}}\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right) \\
&= \frac{\partial}{\partial \lambda}\left(\sum_{n=0}^\infty i^n b_n (1+4\lambda)^{n/2} H_n\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right) \\
&= \sum_{n=0}^\infty i^n b_n \left[4\frac{n}{2}(1+4\lambda)^{n/2-1} H_n\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right. \\
&\qquad\qquad \left. - (1+4\lambda)^{n/2} \frac{4t}{2(1+4\lambda)^{3/2}} H_n'\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right] \\
&= \sum_{n=0}^\infty i^n b_n (1+4\lambda)^{n/2} \\
&\quad \times \left[\frac{1}{1+4\lambda}\left(-H_n''\left(\frac{t}{\sqrt{1+4\lambda}}\right) + \frac{2t}{\sqrt{1+4\lambda}} H_n'\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right)\right. \\
&\qquad\qquad \left. - \frac{2t}{(1+4\lambda)^{3/2}} H_n'\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right]
\end{aligned}$$

$$= -\sum_{n=0}^{\infty} i^n b_n (1+4\lambda)^{n/2} \frac{\partial^2}{\partial t^2}\left(H_n\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right)$$
$$= -\frac{\partial^2}{\partial t^2}\left(X^{\mathcal{H}}_{\sqrt{1+4\lambda}}\left(\frac{t}{\sqrt{1+4\lambda}}\right)\right) = -\frac{\partial^2 \varXi_\lambda(t)}{\partial t^2},$$

recovering (2.52) as expected. (Incidentally, at the heart of this calculation is the simple observation that each of the two-variable functions $h_n(\tau, x) = \tau^{n/2} H_n(-x/\sqrt{\tau})$ solves the time-reversed heat equation $(h_n)_\tau = -\frac{1}{4}(h_n)_{xx}$. With a bit of hindsight, this fact coupled with knowledge of (2.52) could have been seen as yet another clue foreshadowing the connection we made explicit in Theorem 2.9.)

One reason why the above derivation was worth noting is that it has a nice analogue in the context of the expansion of the Riemann xi function in the orthogonal polynomial family $(f_n)_{n=0}^{\infty}$—see Theorem 3.7 in Section 3.4.

3. Expansion of $\varXi(t)$ in the polynomials f_n. Recall that in the Introduction we discussed a family of polynomials $(f_n)_{n=0}^{\infty}$ defined as

$$f_n(x) = P_n^{(3/4)}(x; \pi/2) = \frac{(3/2)_n}{n!} i^n \, {}_2F_1\left(-n, \frac{3}{4} + ix; \frac{3}{2}; 2\right),$$

where $P_n^{(\lambda)}(x; \phi)$ denotes the Meixner–Pollaczek polynomial with parameters λ, ϕ. The polynomials f_n form a family of orthogonal polynomials with respect to the weight function $|\varGamma(3/4+ix)|^2$ on $\mathbb{R}$. Their properties are summarized in Section A.2. Our main goal now is to derive the expansion (1.16) for $\varXi(t)$ in the (trivially rescaled) orthogonal polynomials $f_n(t/2)$, which we refer to as the *f_n-expansion*, and to investigate some of its key properties. After proving two main results about the existence of the expansion and the asymptotic behavior of the coefficients, we will see that thinking about the f_n-expansion leads to a natural family of approximations to $\varXi(t)$ arising out of the Poisson flow of the orthogonal polynomial family $(f_n)_{n=0}^{\infty}$. The ideas in this section will also prepare the ground for additional theory which will be developed in Section 4.

3.1. Main results. We start by identifying the numbers c_{2n} that will play the role of the coefficients in the f_n-expansion. More generally, we define numbers $(c_n)_{n=0}^{\infty}$ by

$$c_n = 2\sqrt{2} \int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^n dx. \tag{3.1}$$

The integral converges absolutely, by (2.5)–(2.6). Moreover, the functional equation (1.9) implies through a trivial change of variables $u = 1/x$ that

$$\int_0^1 \frac{\omega(x)}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^n dx = (-1)^n \int_1^\infty \frac{\omega(u)}{(u+1)^{3/2}} \left(\frac{u-1}{u+1}\right)^n du. \tag{3.2}$$

It follows that $c_{2n+1} = 0$ for all n, and that the even-indexed numbers c_{2n} can be alternatively expressed as

$$c_{2n} = 4\sqrt{2} \int_1^\infty \frac{\omega(x)}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^{2n} dx. \tag{3.3}$$

Since the integrand in (3.3) is positive on $(1, \infty)$, the numbers c_{2n} are positive.

With these preliminary remarks, we can formulate the main result on the expansion (1.16).

THEOREM 3.1 (Infinite series expansion for $\Xi(t)$ in the polynomials f_n). *The Riemann xi function has the infinite series representation*

$$\Xi(t) = \sum_{n=0}^\infty (-1)^n c_{2n} f_{2n}(t/2), \tag{3.4}$$

which converges uniformly on compacts for all $t \in \mathbb{C}$. More precisely, for any compact set $K \subset \mathbb{C}$ there exist constants $C_1, C_2 > 0$ depending on K such that

$$\left| \Xi(t) - \sum_{n=0}^N (-1)^n c_{2n} f_{2n}\left(\frac{t}{2}\right) \right| \le C_1 e^{-C_2\sqrt{N}} \tag{3.5}$$

for all $N \ge 0$ and $t \in K$.

We will also prove a formula describing the asymptotic behavior of the coefficient sequence c_{2n}.

THEOREM 3.2 (Asymptotic formula for the coefficients c_{2n}). *The asymptotic behavior of c_{2n} for large n is given by*

$$c_{2n} = (1 + O(n^{-1/10}))16\sqrt{2}\,\pi^{3/2}\sqrt{n}\exp(-4\sqrt{\pi n}) \tag{3.6}$$

as $n \to \infty$.

A corollary of the above results, analogous to Corollary 2.2 and with an analogous proof, is the following.

COROLLARY 3.3. *The coefficients c_n can be alternatively expressed as*

$$c_n = (-i)^n \frac{\sqrt{2}\,n!}{\pi^{3/2}(3/2)_n} \int_{-\infty}^\infty \Xi(t) f_n\left(\frac{t}{2}\right) \left|\Gamma\left(\frac{3}{4} + \frac{it}{2}\right)\right|^2 dt. \tag{3.7}$$

3.2. Proof of Theorem 3.1. The next two lemmas establish technical bounds that will be useful for our analysis and play a similar role to the one played in the previous section by Lemmas 2.4 and 2.6.

LEMMA 3.4. *The polynomials $f_n(x)$ satisfy the bound*

$$|f_n(x)| \le C_1 e^{C_2 n^{1/3}} \tag{3.8}$$

for all $n \ge 0$, uniformly as x ranges over any compact set $K \subset \mathbb{C}$, with $C_1, C_2 > 0$ being constants that depend on K but not on n.

Proof. Fix the compact $K \subset \mathbb{C}$, and denote $M = 2\max_{x\in K}|x|$. Fix an integer $N_0 \ge \max(4, (3M)^3)$. Let $C_1, C_2 > 0$ be constants for which (3.8) holds for all $x \in K$ and $0 \le n \le N_0$, and such that $C_2 \ge 1$. Note that for all $n \ge N_0$ we have $n^{1/3} - (n-2)^{1/3} \ge \frac{2}{3n^{2/3}}$, which implies that

$$e^{-C_2(n^{1/3}-(n-2)^{1/3})} \le e^{-(n^{1/3}-(n-2)^{1/3})} \le 1 - \frac{1}{3n^{2/3}} \tag{3.9}$$

(since $e^{-x} \le 1 - x/2$ if $0 \le x \le 1$). Then, assuming by induction that we have proved the bound (3.8) for all cases up to $n-1$, in the nth case (where $n > N_0$) we can use the recurrence (A.13) and (3.9) to write that, for all $x \in K$,

$$\begin{aligned}
|f_n(x)| &\le \frac{2|x|}{n}|f_{n-1}(x)| + \left(1 - \frac{1}{2n}\right)|f_{n-2}(x)| \\
&\le \frac{M}{n}C_1 e^{C_2(n-1)^{1/3}} + \left(1 - \frac{1}{2n}\right)C_1 e^{C_2(n-2)^{1/3}} \\
&\le C_1 e^{C_2 n^{1/3}}\left[\frac{M}{n}e^{-C_2(n^{1/3}-(n-1)^{1/3})} + \left(1 - \frac{1}{2n}\right)e^{-C_2(n^{1/3}-(n-2)^{1/3})}\right] \\
&\le C_1 e^{C_2 n^{1/3}}\left[\frac{M}{n} + \left(1 - \frac{1}{2n}\right)\left(1 - \frac{1}{3n^{2/3}}\right)\right] \\
&\le C_1 e^{C_2 n^{1/3}}\left[\frac{1}{3n^{2/3}} + \left(1 - \frac{1}{3n^{2/3}}\right)\right] = C_1 e^{C_2 n^{1/3}}.
\end{aligned}$$

This completes the inductive step. ∎

LEMMA 3.5. *For any number $B \ge 1$ there is a constant $C > 0$ such that*

$$\int_1^\infty e^{-Bx}\left(\frac{x-1}{x+1}\right)^n dx \le Ce^{-2\sqrt{Bn}} \tag{3.10}$$

for all $n \ge 0$.

Proof. The integral can be expressed as

$$\int_1^\infty \exp(\psi_n(x))\,dx,$$

where we define

$$\psi_n(x) = -Bx + n\log\left(\frac{x-1}{x+1}\right). \tag{3.11}$$

By solving the equation $\psi_n'(x) = 0$, it is easy to check that $\psi_n(x)$ has a unique global maximum point x_n in $[1,\infty)$, namely

$$0 = \psi_n'(x_n) = -B + \frac{2n}{x_n^2 - 1} \iff x_n = \sqrt{\frac{2n}{B} + 1},$$

which asymptotically as $n \to \infty$ behaves as

$$x_n = \sqrt{\frac{2n}{B}} + O\left(\frac{1}{\sqrt{n}}\right).$$

The value at the maximum point is

$$\begin{aligned}\psi_n(x_n) &= -Bx_n + n\log\left(\frac{x_n - 1}{x_n + 1}\right) = -Bx_n + n\log\left(\frac{1 - 1/x_n}{1 + 1/x_n}\right)\\ &= -\sqrt{2Bn} + O\left(\frac{1}{\sqrt{n}}\right) + n\left(-2\cdot\frac{1}{x_n} + O\left(\frac{1}{x_n^3}\right)\right)\\ &= -2\sqrt{2Bn} + O\left(\frac{1}{\sqrt{n}}\right)\end{aligned}$$

as $n \to \infty$. We conclude that

$$\begin{aligned}\int_1^\infty \exp(\psi_n(x))\,dx &= \int_1^{2x_n} \exp(\psi_n(x))\,dx + \int_{2x_n}^\infty \exp(\psi_n(x))\,dx\\ &\le 2x_n \exp(\psi_n(x_n)) + \int_{2x_n}^\infty e^{-Bx}\,dx\\ &= \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)2\sqrt{\frac{2n}{B}}\exp(-2\sqrt{2Bn}) + \frac{1}{B}e^{-2Bx_n}\\ &= O(e^{-2\sqrt{Bn}})\end{aligned}$$

as $n \to \infty$, as claimed. ■

Denote $s = 1/2 + it$, and observe that with this substitution the Mellin transform representation (1.10) for $\xi(s)$ becomes the statement that

$$\Xi(t) = \int_0^\infty \omega(x) x^{-3/4+it/2}\,dx.$$

The idea behind the expansion (3.4) is the simple yet powerful fact that the integration kernel $x^{-3/4+it/2}$ can be expanded in a very specific way in an infinite series related to the generating function (A.15). More precisely, for any $x > 0$ we have

$$x^{s/2-1} = x^{-3/4+it/2} = \frac{2\sqrt{2}}{(x+1)^{3/2}}\left(\frac{2x}{x+1}\right)^{-3/4+it/2}\left(\frac{2}{x+1}\right)^{-3/4-it/2} \tag{3.12}$$
$$= \frac{2\sqrt{2}}{(x+1)^{3/2}}\cdot\left((1-iz)^{-3/4+it/2}(1+iz)^{-3/4-it/2}\right)\Big|_{z=i\frac{x-1}{x+1}}$$
$$= \frac{2\sqrt{2}}{(x+1)^{3/2}}\sum_{n=0}^{\infty} f_n\left(\frac{t}{2}\right)\left(i\frac{x-1}{x+1}\right)^n$$
$$= \frac{2\sqrt{2}}{(x+1)^{3/2}}\sum_{n=0}^{\infty} i^n f_n\left(\frac{t}{2}\right)\left(\frac{x-1}{x+1}\right)^n.$$

One can now get (3.4) as a formal identity by multiplying the first and last expressions in (3.12) by $\omega(x)$ and integrating both sides over $(0,\infty)$, then using the fact that the odd-indexed coefficients c_{2n+1} vanish.

To rigorously justify this formal calculation and obtain the more precise rate of convergence estimate (3.5), we now make use of the technical bounds from Lemmas 3.4 and 3.5. Using the above infinite series representation of the kernel $x^{-3/4+it/2}$, we see that

$$\left|\Xi(t) - \sum_{n=0}^{N}(-1)^{2n}c_{2n}f_{2n}\left(\frac{t}{2}\right)\right| = \left|\Xi(t) - \sum_{n=0}^{2N} i^n c_n f_n\left(\frac{t}{2}\right)\right|$$
$$= \left|\int_0^\infty \omega(x)\left(x^{-3/4+it/2} - \frac{2\sqrt{2}}{(x+1)^{3/2}}\sum_{n=0}^{2N} f_n\left(\frac{t}{2}\right)\left(i\frac{x-1}{x+1}\right)^n\right)dx\right|$$
$$\le \int_0^\infty \omega(x)\left|x^{-3/4+it/2} - \frac{2\sqrt{2}}{(x+1)^{3/2}}\sum_{n=0}^{2N} f_n\left(\frac{t}{2}\right)\left(i\frac{x-1}{x+1}\right)^n\right|dx$$
$$= 2\sqrt{2}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left|\sum_{n=2N+1}^{\infty} f_n\left(\frac{t}{2}\right)\left(i\frac{x-1}{x+1}\right)^n\right|dx$$
$$\le 2\sqrt{2}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\sum_{n=2N+1}^{\infty}\left|f_n\left(\frac{t}{2}\right)\right|\cdot\left|i\frac{x-1}{x+1}\right|^n dx$$
$$\le 2\sqrt{2}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\sum_{n=2N+1}^{\infty} C_1 e^{C_2 n^{1/3}}\left|\frac{x-1}{x+1}\right|^n dx$$
$$= 2\sqrt{2}\sum_{n=2N+1}^{\infty} C_1 e^{C_2 n^{1/3}}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left|\frac{x-1}{x+1}\right|^n dx$$
$$= 4\sqrt{2}\sum_{n=2N+1}^{\infty} C_1 e^{C_2 n^{1/3}}\int_1^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^n dx,$$

where C_1, C_2 are the constants from Lemma 3.4 (associated with the compact set K over which we are allowing t to range); the last step follows from (3.2). Now note that, by (2.5), $\frac{\omega(x)}{(x+1)^{3/2}} = O(\sqrt{x}\, e^{-\pi x}) = O(e^{-\pi x/2})$ as $x \to \infty$, so we can apply Lemma 3.5 (with $B = \pi/2$) to the integrals, to find that the last expression in the above chain of inequalities is bounded by

$$4\sqrt{2} \sum_{n=2N+1}^{\infty} C_1 e^{C_2 n^{1/3}} \cdot C e^{-2\sqrt{\pi n/2}},$$

x and this is easily seen to be $O(e^{-\sqrt{\pi N}})$ as $N \to \infty$. This proves (3.5) and completes the proof of Theorem 3.1. ■

3.3. Proof of Theorem 3.2. Define a function $\phi(x)$, and numbers Z_n and ε_n, by

$$\begin{aligned} \phi(x) &= \frac{\pi x(2\pi x - 3)}{(x+1)^{3/2}}, \\ Z_n &= \int_1^\infty \phi(x) e^{-\pi x} \left(\frac{x-1}{x+1}\right)^{2n} dx, \\ \varepsilon_n &= \int_1^\infty \left(\frac{\omega(x)}{(x+1)^{3/2}} - \phi(x) e^{-\pi x}\right) \left(\frac{x-1}{x+1}\right)^{2n} dx, \end{aligned}$$

so that c_{2n} in (3.3) can be rewritten as $c_{2n} = 4\sqrt{2}\,(Z_n + \varepsilon_n)$. We consider separately the asymptotic behavior of Z_n and ε_n. For ε_n, note that

$$\left| \frac{\omega(x)}{(x+1)^{3/2}} - \phi(x) e^{-\pi x} \right| = O(e^{-3\pi x}) \quad \text{as } x \to \infty, \tag{3.13}$$

by (2.7). Thus, Lemma 3.5 implies that

$$|\varepsilon_n| = O(e^{-2\sqrt{6\pi n}}) \quad \text{as } n \to \infty. \tag{3.14}$$

The main asymptotic contribution to c_{2n} comes from Z_n, and can be found using Laplace's method. Start by rewriting Z_n as

$$Z_n = \int_1^\infty \phi(x) \exp(\psi_{2n}(x))\, dx,$$

where $\psi_n(x)$ is the function defined in (3.11) with $B = \pi$. Noting that, as was discussed in the proof of Lemma 3.5, $\psi_{2n}(x)$ has a unique global maximum point at

$$\tau_n := x_{2n} = \sqrt{\frac{4n}{\pi} + 1} = \sqrt{\frac{4n}{\pi}} + O\left(\frac{1}{\sqrt{n}}\right) \quad \text{as } n \to \infty,$$

we further split this integral up into three parts: $Z_n = Z_n^{(1)} + Z_n^{(2)} + Z_n^{(3)}$ with

$$Z_n^{(1)} = \int_1^{\tau_n - n^{3/10}} \phi(x) \exp(\psi_{2n}(x))\, dx, \tag{3.15}$$

$$Z_n^{(2)} = \int_{I_n} \phi(x) \exp(\psi_{2n}(x))\, dx, \tag{3.16}$$

$$Z_n^{(3)} = \int_{\tau_n + n^{3/10}}^{\infty} \phi(x) \exp(\psi_{2n}(x))\, dx, \tag{3.17}$$

where I_n denotes the interval $[\tau_n - n^{3/10}, \tau_n + n^{3/10}]$.

The following calculus facts are straightforward to check; their verification is left to the reader:

(1) $\phi(x)$ is increasing on $[1, \infty)$.
(2) $\psi_{2n}(x)$ is increasing on $[1, \tau_n]$ and decreasing on $[\tau_n, \infty)$.
(3) $\psi_{2n}(x)$ is concave on $[1, \infty)$.
(4) We have the asymptotic relations

$$V_n := \psi_{2n}(\tau_n) = -\pi\tau_n + 2n \log\left(\frac{\tau_n - 1}{\tau_n + 1}\right) = -4\sqrt{\pi n} + O\left(\frac{1}{\sqrt{n}}\right),$$

$$D_n := -\psi_{2n}''(\tau_n) = \frac{\pi^2}{2n}\tau_n = \pi^{3/2}\frac{1}{\sqrt{n}} + O\left(\frac{1}{n^{3/2}}\right),$$

$$E_n := \phi(\tau_n) = 2\sqrt{2}\pi^{7/4} n^{1/4} + O\left(\frac{1}{n^{1/4}}\right),$$

$$K_n := \psi_{2n}'(\tau_n + n^{3/10}) = -\pi^{3/2} n^{-1/5} + O\left(\frac{1}{n^{2/5}}\right),$$

as $n \to \infty$.

(5) We have the relation $\psi_{2n}'''(x) = 8n(3x^2 + 1)/(x^2 - 1)^3$. Consequently,

$$\sup_{x \in I_n} |\psi_{2n}'''(x)| = O\left(\frac{1}{n}\right) \qquad \text{as } n \to \infty,$$

which implies that the Taylor expansion of $\psi_{2n}(x)$ around $x = \tau_n$ can be written as

$$\psi_{2n}(x) = V_n - \frac{1}{2}D_n(x - \tau_n)^2 + O\left(\frac{|x - \tau_n|^3}{n}\right) \qquad (x \in I_n),$$

where the constant implicit in the big-O term does not depend on x or n.

(6) We have

$$\sup_{x \in I_n} \left| \frac{\phi(x)}{E_n} - 1 \right| = O\left(\frac{1}{n^{1/5}}\right) \qquad \text{as } n \to \infty.$$

We now estimate the integrals (3.15)–(3.17). For $Z_n^{(1)}$, since $\phi(x)$ and $\psi_{2n}(x)$ are increasing on $[1, \tau_n]$, we have

$$\begin{aligned}(3.18)\qquad |Z_n^{(1)}| &\le (\tau_n - n^{3/10} - 1)\phi(\tau_n - n^{3/10}) \exp(\psi_{2n}(\tau_n - n^{3/10})) \\ &\le O(n^{3/4}) \exp\left(V_n - \frac{1}{2}D_n n^{3/5} + O\left(\frac{n^{9/10}}{n}\right)\right) = O\left(\frac{1}{n^2} e^{-4\sqrt{\pi n}}\right)\end{aligned}$$

as $n \to \infty$.

For $Z_n^{(3)}$, we use the fact that

$$\psi_{2n}(x) \le \psi_{2n}(\tau_n + n^{3/10}) + K_n(x - \tau_n - n^{3/10})$$

for all $x \ge \tau_n + n^{3/10}$ (which follows from the concavity of $\psi_{2n}(x)$) to write

(3.19)

$$\begin{aligned}|Z_n^{(3)}| &\le \int_{\tau_n + n^{3/10}}^{\infty} \phi(x) \exp[\psi_{2n}(\tau_n + n^{3/10}) + K_n(x - \tau_n - n^{3/10})]\, dx \\ &\le \exp\left[V_n - \frac{1}{2}D_n n^{3/5} + O\left(\frac{n^{9/10}}{n}\right)\right] \\ &\quad \times \int_{\tau_n + n^{3/10}}^{\infty} O(\sqrt{x}) \exp\left[-\left(1 + O\left(\frac{1}{n^{1/5}}\right)\right)\right. \\ &\qquad\qquad \left. \times\, \pi^{3/2} n^{-1/5}(x - \tau_n - n^{3/10})\right] dx \\ &= e^{-4\sqrt{\pi n}} O(e^{-n^{1/20}}) = O\left(\frac{1}{n^2} e^{-4\sqrt{\pi n}}\right).\end{aligned}$$

Finally, to obtain the asymptotics of $Z_n^{(2)}$, we make the change of variables $u = \sqrt{D_n}\,(x - \tau_n)$ in the integral (3.16), to get

(3.20)

$$\begin{aligned}Z_n^{(2)} &= \int_{-\sqrt{D_n} n^{3/10}}^{\sqrt{D_n} n^{3/10}} \phi\left(\tau_n + \frac{u}{\sqrt{D_n}}\right) \exp\left(\psi_{2n}\left(\tau_n + \frac{u}{\sqrt{D_n}}\right)\right) \frac{du}{\sqrt{D_n}} \\ &= \frac{1}{\sqrt{D_n}} \int_{-\sqrt{D_n} n^{3/10}}^{\sqrt{D_n} n^{3/10}} \phi\left(\tau_n + \frac{u}{\sqrt{D_n}}\right) \exp\left[V_n - \frac{1}{2}u^2 + O\left(\frac{|u|^3}{n D_n^{3/2}}\right)\right] du \\ &= \left(1 + O\left(\frac{1}{n^{1/4}}\right)\right) \pi^{-3/4} n^{1/4} \times \left(1 + O\left(\frac{1}{n^{1/5}}\right)\right) E_n \\ &\quad \times \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right) e^{-4\sqrt{\pi n}} \int_{-\sqrt{D_n} n^{3/10}}^{\sqrt{D_n} n^{3/10}} \exp\left[-\frac{1}{2}u^2 + O\left(\frac{1}{n^{1/10}}\right)\right] du\end{aligned}$$

$$= \left(1 + O\left(\frac{1}{n^{1/10}}\right)\right)\pi^{-3/4}n^{1/4} \times 2\sqrt{2}\,\pi^{7/4}n^{1/4} \times e^{-4\sqrt{\pi n}}$$
$$\times \left(\sqrt{2\pi} - O\left(\exp\left(-\frac{1}{2}D_n n^{3/5}\right)\right)\right)$$
$$= \left(1 + O\left(\frac{1}{n^{1/10}}\right)\right)4\pi^{3/2}n^{1/2}e^{-4\sqrt{\pi n}},$$

where we once again used (2.39) to account for the error arising from adding the tails of the Gaussian integral.

Since $c_{2n} = 4\sqrt{2}\,(\varepsilon_n + Z_n^{(1)} + Z_n^{(2)} + Z_n^{(3)})$, combining (3.14), (3.18), (3.19) and (3.20) gives the asymptotic formula (3.6). The proof of Theorem 3.2 is complete. ■

3.4. The Poisson flow associated with the f_n-expansion. Motivated by the developments of Section 2.5, we now consider the Poisson flow (2.48) associated with the family $(f_n)_{n=0}^{\infty}$ of orthogonal polynomials, which in this section we will denote by $\mathcal{F}$. Recall that in the case of the Hermite expansion, we showed that the Poisson flow could be understood as the family of Fourier transforms of functions obtained from the function $\varPhi(x)$ by performing a simple operation (refer to (2.51)). One might wonder if something similar (or perhaps even more interesting) happens in the case of the Poisson flow associated with the family $\mathcal{F}$. The answer is given in the following result.

THEOREM 3.6 (Mellin transform representation of the Poisson flow). *For $0 < r < 1$, the function $X_r^{\mathcal{F}}(t)$ has the Mellin transform representation*

$$X_r^{\mathcal{F}}(t) = \int_0^{\infty} \omega_r(x)x^{-3/4+it/2}\,dx \qquad (t \in \mathbb{C}), \tag{3.21}$$

where we define

$$\omega_r(x) = \begin{cases} \dfrac{1+\eta}{\sqrt{1-\eta}}\,\dfrac{1}{\sqrt{1-\eta x}}\,\omega\left(\dfrac{x-\eta}{1-\eta x}\right) & \text{if } \eta < x < 1/\eta, \\ 0 & \text{otherwise}, \end{cases} \tag{3.22}$$

making use of the notation

$$\eta = \frac{1-r}{1+r}. \tag{3.23}$$

Note that the map $x \mapsto \frac{x-\eta}{1-\eta x}$ maps the interval $(\eta, 1/\eta)$ bijectively onto $(0,\infty)$, so the function $\omega_r(x)$ contains the same "frequency information" as $\omega(x)$, but compressed into a finite interval. In particular, a notable feature of this result, which stands in contrast to what we saw in the case of the Poisson flow associated with the Hermite polynomials, is that for $r < 1$ the function $X_r^{\mathcal{F}}(t)$ is now the Fourier transform of a function with bounded support; that is, $X_r^{\mathcal{F}}(t)$ is an entire function of exponential type. It is intriguing to speculate that this might make the problem of understanding where the zeros of $X_r^{\mathcal{F}}(t)$ are located easier than for the case of the original xi function $\Xi(t)$.

Proof of Theorem 3.6. The derivation starts with the formula (2.49). Specializing this to the expansion (3.4) and substituting the defining formula (3.1) for the coefficients c_n, we have

$$\begin{aligned} X_r^{\mathcal{F}}(t) &= \sum_{n=0}^{\infty} i^n c_n r^n f_n\left(\frac{t}{2}\right) \\ &= 2\sqrt{2}\sum_{n=0}^{\infty}\int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^n dx \cdot r^n f_n\left(\frac{t}{2}\right) \\ &= 2\sqrt{2}\int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}} \sum_{n=0}^{\infty} f_n\left(\frac{t}{2}\right)\left(ir\frac{x-1}{x+1}\right)^n dx \\ &= 2\sqrt{2}\int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}} \left(\sum_{n=0}^{\infty} f_n\left(\frac{t}{2}\right) z^n\right)\Bigg|_{z=ir\frac{x-1}{x+1}} dx. \end{aligned}$$

Inside the integrand we have an expression involving the generating function (A.15) of the polynomials $f_n(x)$. Substituting the formula for this generating function (as we did in (3.12), which is essentially the special case $r = 1$ of the current computation) gives

$$\begin{aligned} X_r^{\mathcal{F}}(t) &= 2\sqrt{2}\int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}}\left((1-iz)^{-3/4+it/2}(1+iz)^{-3/4+it/2)}\right)\Bigg|_{z=ir\frac{x-1}{x+1}} dx \\ &= 2\sqrt{2}\int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{1-r+x(1+r)}{x+1}\right)^{-3/4+it/2} \\ &\qquad\qquad\qquad\qquad \times\left(\frac{1+r+x(1-r)}{x+1}\right)^{-3/4-it/2} dx \\ &= 2\sqrt{2}\int_0^{\infty} \omega(x)(1+r)^{-3/4+it/2}\left(x+\frac{1-r}{1+r}\right)^{-3/4+it/2} \\ &\qquad\qquad\qquad\qquad \times(1+r)^{-3/4-it/2}\left(1+\frac{1-r}{1+r}x\right)^{-3/4-it/2} dx \\ &= \frac{2\sqrt{2}}{(1+r)^{3/2}}\int_0^{\infty} \omega(x)\frac{1}{(1+\eta x)^{3/2}}\left(\frac{x+\eta}{1+\eta x}\right)^{-3/4+it/2} dx \\ &= (1+\eta)^{3/2}\int_0^{\infty} \omega(x)\frac{1}{(1+\eta x)^{3/2}}\left(\frac{x+\eta}{1+\eta x}\right)^{-3/4+it/2} dx. \end{aligned}$$

We have thus expressed $X_r^{\mathcal{F}}(t)$ as a sort of modified Mellin transform of $\omega(x)$. But this last integral formula can be transformed to an ordinary Mellin transform by making the change of variables $x = \frac{u-\eta}{1-\eta u}$ in the last integral. The reader can verify without difficulty that this yields the Mellin transform (3.21) of the function given in (3.22). ∎

In the next result we show that the Poisson flow satisfies an interesting dynamical evolution law, analogous to the time-reversed heat equation (2.52) satisfied by the Pólya–de Bruijn flow. In this case the evolution law is not a partial differential equation, but rather a *differential difference equation* (*DDE*). To make the equation homogeneous in the "time" variable, it is most convenient to perform a change of variables, reparametrizing the time variable r by denoting $r = e^{-\tau}$ (with $\tau \geq 0$).

THEOREM 3.7 (Differential difference equation for the Poisson flow). *The function $M(\tau, t) := X_{e^{-\tau}}^{\mathcal{F}}(t)$ satisfies the differential difference equation*

$$\frac{\partial M}{\partial \tau} = \frac{3}{4} M(\tau, t) - \frac{1}{2}\left(\frac{3}{4} - \frac{it}{2}\right) M(\tau, t+2i) - \frac{1}{2}\left(\frac{3}{4} + \frac{it}{2}\right) M(\tau, t-2i) \tag{3.24}$$

for $\tau > 0$, and $t \in \mathbb{C}$.

Proof. The computation is analogous to the derivation of the time-reversed heat equation at the end of Section 2.5, except that instead of using the differential equation satisfied by the Hermite polynomials we use the difference equation (A.14) satisfied by the polynomials $f_n(x)$. We have, again starting with (2.49) with the substitution $r = e^{-\tau}$,

$$\begin{aligned}
\frac{\partial M}{\partial \tau} &= \frac{\partial}{\partial \tau}\left(\sum_{n=0}^{\infty} i^n c_n e^{-n\tau} f_n\left(\frac{t}{2}\right)\right) = \sum_{n=0}^{\infty} i^n c_n (-n) e^{-n\tau} f_n\left(\frac{t}{2}\right) \\
&= \sum_{n=0}^{\infty} i^n c_n e^{-n\tau} \left(\frac{3}{4} f_n\left(\frac{t}{2}\right) - \frac{1}{2}\left(\frac{3}{4} + \frac{it}{2}\right) f_n\left(\frac{t}{2} - i\right)\right. \\
&\qquad\qquad \left. - \frac{1}{2}\left(\frac{3}{4} - \frac{it}{2}\right) f_n\left(\frac{t}{2} + i\right)\right) \\
&= \frac{3}{4} \sum_{n=0}^{\infty} i^n c_n e^{-n\tau} f_n\left(\frac{t}{2}\right) - \frac{1}{2}\left(\frac{3}{4} + \frac{it}{2}\right) \sum_{n=0}^{\infty} i^n c_n e^{-n\tau} f_n\left(\frac{t}{2} - i\right) \\
&\qquad - \frac{1}{2}\left(\frac{3}{4} - \frac{it}{2}\right) \sum_{n=0}^{\infty} i^n c_n e^{-n\tau} f_n\left(\frac{t}{2} + i\right) \\
&= \frac{3}{4} M(\tau, t) - \frac{1}{2}\left(\frac{3}{4} - \frac{it}{2}\right) M(\tau, t+2i) - \frac{1}{2}\left(\frac{3}{4} + \frac{it}{2}\right) M(\tau, t-2i). \quad ∎
\end{aligned}$$

3.5. Evolution of the zeros under the Poisson flow. The differential difference equation (3.24) opens up the way to an analysis of the dynamical evolution of the zeros of the functions $X_r^{\mathcal{F}}(t)$ as a function of r, in a manner analogous to how the time-reversed heat equation (2.52) made it possible to write a system of coupled ODEs satisfied by the Pólya–de Bruijn flow, which played a useful role in the investigations of the de Bruijn–Newman constant (see [9, Lemma 5.18, p. 83]). Our next goal is to derive this evolution law, again using the more convenient time parameter τ. To avoid technicalities involving the behavior of entire functions (and to generalize the question slightly, which also seems potentially useful), we switch in this section from the Riemann xi function to the simpler setting of polynomials.

Let $z_1, \ldots, z_n \in \mathbb{C}$ be distinct complex numbers. Let

$$p(t) = \prod_{k=1}^{n} (t - z_k), \tag{3.25}$$

and consider the function $M_p(\tau, t)$ defined as the solution to the DDE (3.24) with initial condition $M_p(0, t) = p(t)$. To see that such an object exists, write the expansion

$$p(t) = \sum_{k=0}^{n} \gamma_k f_k(t/2)$$

in the linear basis of polynomials $(f_k(t/2))_{k=0}^n$. Then $M_p(\tau, t)$ is given by

$$M_p(\tau, t) = \sum_{k=0}^{n} \gamma_k e^{-k\tau} f_k(t/2) \tag{3.26}$$

(the proof is a repetition of the calculation in the proof of Theorem 3.7 above, with both proofs being based on the simple observation that each of the functions $m_k(\tau, t) = e^{-k\tau} f_k(t/2)$ for $k \geq 0$ is a solution to (3.24)). Proving uniqueness is left as an exercise. We refer to the function $M_p(\tau, t)$ as the *Poisson flow* (*associated with the polynomial family* $\mathcal{F}$) *with initial condition* p.

For any fixed $\tau \in \mathbb{R}$, the function $t \mapsto M_p(\tau, t)$ is a polynomial of degree n with leading coefficient $e^{-n\tau}$ (to see this, compare (3.26) at times τ and 0, taking into account (3.25)). Denote its zeros by $Z_1(\tau), \ldots, Z_n(\tau)$, and note that while they are defined only up to ordering, in the neighborhood of any fixed time τ_0 for which the zeros are distinct one can pick the ordering so that $Z_k(\tau)$ are smooth functions of τ.

THEOREM 3.8 (Evolution equations for the zeros under the Poisson flow). *In the neighborhood of any* τ_0 *as above, the functions* $(Z_k(\tau))_{k=1}^n$ *satisfy the system of coupled ordinary differential equations*

$$\frac{dZ_k}{d\tau} = \frac{1}{2}\Bigg[\left(Z_k + \frac{3i}{2}\right) \prod_{\substack{1\le j\le n\\ j\ne k}} \left(1 + \frac{2i}{Z_k - Z_j}\right) + \left(Z_k - \frac{3i}{2}\right) \prod_{\substack{1\le j\le n\\ j\ne k}} \left(1 - \frac{2i}{Z_k - Z_j}\right)\Bigg] \qquad (1 \le k \le n).$$

Proof. The fundamental relation defining the kth zero Z_k is

$$M_p(\tau, Z_k(\tau)) = 0.$$

Differentiating this with respect to τ gives

$$0 = \frac{d}{d\tau}\big(M_p(\tau, Z_k(\tau))\big) = \frac{\partial M_p}{\partial \tau}(\tau, Z_k(\tau)) + \frac{\partial M_p}{\partial t}(\tau, Z_k(\tau))\frac{dZ_k}{d\tau}$$

(where $\frac{\partial M_p}{\partial t}$ refers to the partial derivative with respect to the second variable). By (3.24), this expands to

$$\begin{aligned}
0 &= \frac{3}{4}M_p(\tau, Z_k) - \frac{1}{2}\left(\frac{3}{4} - \frac{iZ_k}{2}\right)M_p(\tau, Z_k + 2i) \\
&\quad - \frac{1}{2}\left(\frac{3}{4} + \frac{iZ_k}{2}\right)M_p(\tau, Z_k - 2i) + \frac{\partial M_p}{\partial t}(\tau, Z_k(\tau))\frac{dZ_k}{d\tau} \\
&= -\frac{1}{2}\left(\frac{3}{4} - \frac{iZ_k}{2}\right)M_p(\tau, Z_k + 2i) - \frac{1}{2}\left(\frac{3}{4} + \frac{iZ_k}{2}\right)M_p(\tau, Z_k - 2i) \\
&\quad + \frac{\partial M_p}{\partial t}(\tau, Z_k(\tau))\frac{dZ_k}{d\tau}.
\end{aligned}$$

Now, $M_p(\tau, t) = e^{-n\tau}\prod_{j=1}^n (t - Z_j(\tau))$, so

$$\frac{\partial M_p}{\partial t}(\tau, Z_k(\tau)) = e^{-n\tau} \prod_{\substack{1\le j\le n\\ j\ne k}} (Z_k - Z_j).$$

It follows that

$$\begin{aligned}
\frac{dZ_k}{d\tau} &= \frac{1}{2}\,\frac{1}{\frac{\partial M_p}{\partial t}(\tau, Z_k(\tau))}\Bigg[\left(\frac{3}{4} - \frac{iZ_k}{2}\right)M_p(\tau, Z_k + 2i) \\
&\qquad\qquad + \left(\frac{3}{4} + \frac{iZ_k}{2}\right)M_p(\tau, Z_k - 2i)\Bigg] \\
&= \frac{1}{2}\,\frac{\left(\frac{3}{4} - \frac{iZ_k}{2}\right)\prod_{j=1}^n (Z_k + 2i - Z_j) + \left(\frac{3}{4} + \frac{iZ_k}{2}\right)\prod_{j=1}^n (Z_k - 2i - Z_j)}{\prod_{1\le j\le n,\, j\ne k}(Z_k - Z_j)} \\
&= \frac{1}{2}\Bigg[2i\left(\frac{3}{4} - \frac{iZ_k}{2}\right) \prod_{\substack{1\le j\le n\\ j\ne k}} \frac{Z_k + 2i - Z_j}{Z_k - Z_j} \\
&\qquad\qquad + (-2i)\left(\frac{3}{4} + \frac{iZ_k}{2}\right) \prod_{\substack{1\le j\le n\\ j\ne k}} \frac{Z_k - 2i - Z_j}{Z_k - Z_j}\Bigg]
\end{aligned}$$

$$= \frac{1}{2}\Bigg[\left(Z_k + \frac{3i}{2}\right) \prod_{\substack{1\le j\le n\\ j\ne k}} \left(1 + \frac{2i}{Z_k - Z_j}\right) + \left(Z_k - \frac{3i}{2}\right) \prod_{\substack{1\le j\le n\\ j\ne k}} \left(1 - \frac{2i}{Z_k - Z_j}\right)\Bigg],$$

as claimed. ■

Our final result for this section is of a negative sort, illustrating another way in which the Poisson flow associated with the family $\mathcal{F}$ of orthogonal polynomials behaves differently from the Pólya–de Bruijn flow. Specifically, it was mentioned in Section 2.5 that the Pólya–de Bruijn flow preserves the property of hyperbolicity. Our result shows that the Poisson flow associated with the family $\mathcal{F}$ does *not*.

PROPOSITION 3.9. *There exists a polynomial*

$$P(t) = \sum_{k=0}^{n} \gamma_k f_k(t/2),$$

and numbers $\tau_1 > 0$ *and* $\tau_2 < 0$, *such that* $P(t)$ *has only real zeros, but the polynomials* $t \mapsto M_P(\tau_1, t)$ *and* $t \mapsto M_P(\tau_2, t)$ *both have non-real zeros.*

Proof. Take

$$P(t) = (x-2)(x-2.01)(x-4) = \sum_{k=0}^{4} \sigma_k f_k(t/2),$$

where

$$(\sigma_0, \sigma_1, \sigma_2, \sigma_3) = \left(-\frac{5619}{1600}, \frac{83}{25}, -\frac{801}{400}, \frac{3}{4}\right),$$

and $\tau_1 = 0.1$ and $\tau_2 = -0.05$. Direct calculation of the zeros of $M_P(\tau_1, t)$ and $M_P(\tau_2, t)$ verifies the claim. ■

One conclusion from Proposition 3.9 is that there does not seem to be an obvious way to define an analogue of the de Bruijn–Newman constant in the context of the f_n-expansion of the Riemann xi function.

4. Expansion of $\Xi(t)$ in the polynomials g_n. In this section we continue to build on the tools developed in Section 3 in order to derive an infinite series expansion for the Riemann xi function in yet another family of orthogonal polynomials, the family $(g_n(x))_{n=0}^{\infty}$, and study its properties. As we discussed briefly in the Introduction, the polynomials g_n are defined by

$$g_n(x) = p_n\left(x; \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right) = i^n (n+1)\, {}_3F_2\left(-n, n+2, \frac{3}{4} + ix; \frac{3}{2}, \frac{3}{2}; 1\right),$$

where $p_n(x; a, b, c, d)$ denotes the continuous Hahn polynomial with parameters a, b, c, d. They form a family of orthogonal polynomials with respect to the weight function $|\Gamma(3/4+ix)|^4$ on $\mathbb{R}$. Their main properties are summarized in Section A.3.

4.1. Main results. As in Sections 2 and 3, we start by defining a sequence of numbers $(d_n)_{n=0}^\infty$ that will play the role of the coefficients associated with the new expansion. Define

$$d_n = \frac{(3/2)_n}{2^{n-3/2}n!}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^n \times {}_2F_1\left(\frac{n}{2}+\frac{3}{4},\frac{n}{2}+\frac{5}{4};n+2;\left(\frac{x-1}{x+1}\right)^2\right)dx. \tag{4.1}$$

As a first step towards demystifying this somewhat obscure definition, we expand the ${}_2F_1$ term in an infinite series. Momentarily ignoring issues of convergence, we have

$$\begin{aligned} d_n &= \frac{(3/2)_n}{2^{n-3/2}n!}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^n \\ &\qquad\times\left[\sum_{m=0}^\infty \frac{\left(\frac{n}{2}+\frac{3}{4}\right)_m\left(\frac{n}{2}+\frac{5}{4}\right)_m}{m!(n+2)_m}\left(\frac{x-1}{x+1}\right)^{2m}\right]dx \\ &= \frac{(3/2)_n}{2^{n-3/2}n!}\sum_{m=0}^\infty \frac{\left(\frac{n}{2}+\frac{3}{4}\right)_m\left(\frac{n}{2}+\frac{5}{4}\right)_m}{m!(n+2)_m}\int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^{n+2m}dx \\ &= \frac{(3/2)_n}{2^n n!}\sum_{m=0}^\infty \frac{\left(\frac{n}{2}+\frac{3}{4}\right)_m\left(\frac{n}{2}+\frac{5}{4}\right)_m}{m!(n+2)_m}c_{n+2m} \\ &= \frac{n+1}{2^n}\sum_{m=0}^\infty \frac{(3/2)_{n+2m}}{4^m m!(n+m+1)!}c_{n+2m}, \end{aligned} \tag{4.2}$$

where in the last step we use the relation $\left(\frac{n}{2}+\frac{3}{4}\right)_m\left(\frac{n}{2}+\frac{5}{4}\right)_m = \frac{(3/2)_{n+2m}}{2^{2m}(3/2)_n}$. In addition to being an interesting way to express d_n in terms of the coefficients c_k, this suggests a relatively simple way to see that the integral (4.1) converges absolutely (which would also justify the above formal computation); namely, letting

$$c_n' = \int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}}\left|\frac{x-1}{x+1}\right|^n dx,$$

we have the simple relations $c_r' \ge c_{r+1}'$, $c_{2r}' = c_{2r}$, and therefore (using (3.6), or some easy corollary of Lemma 3.5) deduce that $c_r' \le Ke^{-M\sqrt{r}}$ for all $r \ge 0$ and some constants $K, M > 0$. This then gives

$$\int_0^\infty \left|\frac{\omega(x)}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^n {}_2F_1\left(\frac{n}{2}+\frac{3}{4},\frac{n}{2}+\frac{5}{4};n+2;\left(\frac{x-1}{x+1}\right)^2\right)\right|dx \tag{4.3}$$

$$\leq \sum_{m=0}^{\infty} \frac{\left(\frac{n}{2}+\frac{3}{4}\right)_m \left(\frac{n}{2}+\frac{5}{4}\right)_m}{m!(n+2)_m} \int_0^\infty \left| \frac{\omega(x)}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^{n+2m} \right| dx$$

$$= \sum_{m=0}^{\infty} \frac{\left(\frac{n}{2}+\frac{3}{4}\right)_m \left(\frac{n}{2}+\frac{5}{4}\right)_m}{m!(n+2)_m} c'_{n+2m} = \frac{(n+1)!}{(3/2)_n} \sum_{m=0}^{\infty} \frac{(3/2)_{n+2m}}{4^m m!(n+m+1)!} c'_{n+2m}$$

$$\leq K \frac{(n+1)!}{(3/2)_n} \sum_{m=0}^{\infty} \frac{(3/2)_{n+2m}}{4^m m!(n+m+1)!} e^{-M\sqrt{n+2m}}$$

$$\leq 2K \frac{(n+1)!}{(3/2)_n} \sum_{m=0}^{\infty} \frac{(2)_{n+2m}}{2^{2m+1} m!(n+m+1)!} e^{-M\sqrt{n+2m}}$$

$$= 2K \frac{(n+1)!}{(3/2)_n} \sum_{m=0}^{\infty} \frac{1}{2^{2m+1}} \binom{n+2m+1}{m} e^{-M\sqrt{n+2m}}$$

$$\leq 2^{n+1} K \frac{(n+1)!}{(3/2)_n} \sum_{m=0}^{\infty} e^{-M\sqrt{n+2m}} < \infty,$$

establishing the absolute convergence.

We summarize the above observations as a proposition.

Proposition 4.1.

(i) *The integral defining d_n converges absolutely for all $n \geq 0$.*
(ii) $d_{2n+1} = 0$ *for all $n \geq 0$.*
(iii) $d_{2n} > 0$ *for all $n \geq 0$.*
(iv) d_n *can be expressed alternatively in terms of the coefficients c_k as*

$$d_n = \frac{n+1}{2^n} \sum_{m=0}^{\infty} \frac{(3/2)_{n+2m}}{4^m m!(n+m+1)!} c_{n+2m}. \tag{4.4}$$

We are ready to formulate the main results concerning the expansion of $\Xi(t)$ in the polynomials g_n, which are precise analogues of Theorems 2.1 and 2.7 in Section 2 and Theorems 3.1 and 3.2 in Section 3.

Theorem 4.2 (Infinite series expansion for $\Xi(t)$ in the polynomials g_n). *The Riemann xi function has the infinite series representation*

$$\Xi(t) = \sum_{n=0}^{\infty} (-1)^n d_{2n} g_{2n}(t/2), \tag{4.5}$$

which converges uniformly on compacts for all $t \in \mathbb{C}$. More precisely, for any compact set $K \subset \mathbb{C}$ there exist constants $C_1, C_2 > 0$ depending on K such that

$$\left| \Xi(t) - \sum_{n=0}^{N} (-1)^n d_{2n} g_{2n}(t/2) \right| \leq C_1 e^{-C_2 N^{2/3}} \tag{4.6}$$

for all $N \geq 0$ and $t \in K$.

Theorem 4.3 (Asymptotic formula for the coefficients d_{2n}). *The asymptotic behavior of d_{2n} for large n is given by*

$$d_{2n} = (1 + O(n^{-1/10}))Dn^{4/3} \exp(-En^{2/3}) \tag{4.7}$$

as $n \to \infty$, where D, E are constants given by

$$D = \frac{128 \times 2^{1/3}\pi^{2/3}e^{-2\pi/3}}{\sqrt{3}}, \qquad E = 3(4\pi)^{1/3}. \tag{4.8}$$

As in Sections 2 and 3, we note the fact that the coefficients d_n can be computed as inner products in the L^2-space $L^2(\mathbb{R}, |\Gamma(3/4 + it/2)|^4)$.

Corollary 4.4. *The coefficients d_n can be alternatively expressed as*

$$d_n = \frac{8}{\pi^3}(-i)^n \int_{-\infty}^{\infty} \Xi(t) g_n\left(\frac{t}{2}\right)\left|\Gamma\left(\frac{3}{4} + \frac{it}{2}\right)\right|^4 dt. \tag{4.9}$$

Proof. Repeat the arguments leading to Corollaries 2.2 and 3.3. ∎

4.2. Proof of Theorem 4.2. The next two lemmas are analogues of Lemmas 2.4 and 2.6 in Section 2 and Lemmas 3.4 and 3.5 in Section 3.

Lemma 4.5. *The polynomials $g_n(x)$ satisfy the bound*

$$|g_n(x)| \le C_1 e^{C_2 n^{1/3}} \tag{4.10}$$

for all $n \ge 0$, uniformly as x ranges over any compact set $K \subset \mathbb{C}$, with $C_1, C_2 > 0$ being constants that depend on K but not on n.

Proof. This is identical to the proof of Lemma 3.4, except that the use of the recurrence relation (A.13) is replaced by the analogous relation (A.22) for the sequence $g_n(x)$, with the result that some small modifications need to be made to the constants in the proof. We leave the details as an exercise. Alternatively, the estimate can also be derived from [13, Theorem 1], which gives a precise asymptotic approximation for the continuous Hahn polynomials. ∎

Lemma 4.6. *There exist constants $J_1, J_2 > 0$ such that for all $n \ge 0$,*

$$\frac{1}{2^n}\int_0^{\infty} \frac{\omega(x)}{(x+1)^{3/2}}\left|\left(\frac{x-1}{x+1}\right)^n {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right)\right| dx \le J_1 e^{-J_2 n^{2/3}}. \tag{4.11}$$

Proof. Note that this is a stronger version of the finiteness bound (4.3) that makes explicit the dependence of the bound on n. To prove it, we refer back to the penultimate line of (4.3) and proceed from there a bit more economically than before. Multiplying by $1/2^n$ and using the trivial fact that $(n+1)!/(3/2)_n \le 2n$, we find that the integral in (4.11) (together with the leading factor of $1/2^n$) is bounded from above by

$$\begin{aligned} 4Kn \sum_{m=0}^{\infty} \frac{1}{2^{n+2m+1}} \binom{n+2m+1}{m} e^{-M\sqrt{n+2m}} \\ = 4Kn\Bigg[\sum_{m \le \frac{1}{8M^{2/3}} n^{4/3}} \frac{1}{2^{n+2m+1}} \binom{n+2m+1}{m} e^{-M\sqrt{n+2m}} \\ + \sum_{m > \frac{1}{8M^{2/3}} n^{4/3}} e^{-M\sqrt{n+2m}} \Bigg] \end{aligned}$$

(with the same constants K, M appearing in (4.3)). We will show that each of the two sums in this last expression satisfies a bound of the sort we need. For the second sum, observe that it is bounded by the integral

$$\int_{\frac{1}{8M^{2/3}} n^{4/3} - 1}^{\infty} e^{-M\sqrt{n+2x}}\, dx,$$

and this integral is $O\big(\exp\big(-\frac{M^{2/3}}{2} n^{2/3}\big)\big)$, by the relation

$$\int_A^{\infty} e^{-M\sqrt{n+2x}} = \frac{1}{M^2}(M\sqrt{n+2A}+1)e^{-M\sqrt{n+2A}}.$$

To estimate the first sum, we claim that the terms in that sum are increasing as a function of m for all large enough (but fixed) n; this would imply that the sum is bounded for large n by $\frac{1}{8M^{2/3}} n^{4/3}$ times the last term, which in turn is at most $O\big(\exp\big(-\frac{M^{2/3}}{2} n^{2/3}\big)\big)$, and hence, when combined with the estimates above, would imply the assertion of the lemma.

To prove the claim, observe that the ratio of successive terms in the sum is

$$\begin{aligned} \frac{\frac{1}{2^{n+2m+3}} \binom{n+2m+3}{m+1} e^{-M\sqrt{n+2m+2}}}{\frac{1}{2^{n+2m+1}} \binom{n+2m+1}{m} e^{-M\sqrt{n+2m}}} \\ = \frac{(n+2m+2)(n+2m+3)}{4(m+1)(n+m+2)} e^{M(\sqrt{n+2m}-\sqrt{n+2m+2})} \\ \ge \frac{(m+n/2)^2}{(m+1)(m+n+2)} \left(1 - \frac{M}{\sqrt{m+n/2}}\right) \\ = \frac{(m+n/2)^2}{(m+n/2)^2 - (n^2/4 - 3m - n - 2)} \left(1 - \frac{M}{\sqrt{m+n/2}}\right). \end{aligned} \tag{4.12}$$

Our claim is equivalent to the statement that, under the assumption $m \le \frac{1}{8M^{2/3}} n^{4/3}$, the last expression in (4.12) is ≥ 1. Equivalently, we need to show that

$$1-\frac{n^2/4-3m-n-2}{(m+n/2)^2} \le 1-\frac{M}{\sqrt{m+n/2}} \tag{4.13}$$

for those values of m. This reduces after some further simple algebra to verifying the inequality

$$m+\frac{n}{2} \le \frac{1}{M^{2/3}}\left(\frac{n^2}{4}-3m-n-2\right)^{2/3}. \tag{4.14}$$

To check this, assume that n is large enough so that the inequalities

$$3\frac{1}{8M^{2/3}}n^{4/3}+n+2 \le \frac{n^2}{8}, \qquad \frac{n}{2} \le \frac{1}{8M^{2/3}}n^{4/3} \tag{4.15}$$

are satisfied. Then, together with our assumption on m, this also implies

$$\frac{n^2}{8} \le \frac{n^2}{4}-3m-n-2,$$

and therefore also that

$$\begin{aligned} m+\frac{n}{2} &\le \frac{1}{8M^{2/3}}n^{4/3}+\frac{1}{8M^{2/3}}n^{4/3} = \frac{1}{4M^{2/3}}n^{4/3} = \frac{1}{M^{2/3}}\left(\frac{n^2}{8}\right)^{2/3} \\ &\le \frac{1}{M^{2/3}}\left(\frac{n^2}{4}-3m-n-2\right)^{2/3}. \end{aligned}$$

This verifies (4.14), hence also (4.13), for all n satisfying (4.15) (which clearly includes all values of n larger than some fixed N_0), and therefore finishes the proof of the claim and also of the lemma. ■

We need one final bit of preparation before proving Theorem 4.2. Recall that in the proof of Theorem 3.1, a key idea was the observation that the integration kernel $x^{s/2-1}$ can be related to the generating function of the polynomials $f_n(t/2)$. The next lemma shows a way of representing the same generating function as an infinite series involving the polynomials $g_n(t/2)$.

LEMMA 4.7. *For $w \in \mathbb{C}$ and $|z| < 1$, we have the identity*

$$\sum_{n=0}^{\infty} f_n(w)z^n = \sum_{n=0}^{\infty} \frac{(3/2)_n}{2^n n!} g_n(w)\ {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; -z^2\right) z^n.$$

Proof. Using the relation (A.27) expressing the polynomial f_n in terms of the g_k's, we can write

$$\begin{aligned} &\sum_{n=0}^{\infty} f_n(w)z^n \\ &= \sum_{n=0}^{\infty}\left(\frac{(3/2)_n}{2^n(n+1)!}\sum_{m=0}^{\lfloor n/2\rfloor}(-1)^m(n-2m+1)\binom{n+1}{m} g_{n-2m}(w)\right) z^n. \end{aligned} \tag{4.16}$$

The claim will follow by suitably rearranging the terms in this double summation. First, let us check that this is permitted by showing that the sum is in fact absolutely convergent. Indeed, using Lemma 4.5 to bound $|g_{n-2m}(w)|$ (with w being fixed and the resulting constants C_1, C_2 depending on w but not on n, m), we see that

$$\begin{aligned}\sum_{n=0}^{\infty}\sum_{m=0}^{\lfloor n/2\rfloor} \frac{(3/2)_n}{2^n(n+1)!}\left|(-1)^m(n-2m+1)\binom{n+1}{m}g_{n-2m}(w)\right|\cdot|z|^n \\ \le \sum_{n=0}^{\infty}\frac{(3/2)_n}{2^n(n+1)!}(n+1)2^{n+1}\times C_1 e^{C_2 n^{1/3}}|z|^n \\ = 2C_1\sum_{n=0}^{\infty}(n+1)e^{C_2 n^{1/3}}|z|^n < \infty.\end{aligned}$$

With absolute convergence established, we can rewrite the double sum in (4.16), introducing a new summation index $k = n-2m$ in place of n, as

$$\begin{aligned}&\sum_{k=0}^{\infty}\sum_{m=0}^{\infty}\frac{(3/2)_{k+2m}}{2^{k+2m}(k+2m+1)!}(-1)^m(k+1)\binom{k+2m+1}{m}g_k(w)z^{k+2m} \\ &= \sum_{k=0}^{\infty}\frac{(3/2)_k}{2^k k!}g_k(w)z^k\left(\sum_{m=0}^{\infty}\frac{(-z^2)^m}{m!}\,\frac{(3/2)_{k+2m}}{(3/2)_k 2^{2m}}\,\frac{(k+1)!}{(k+m+1)!}\right) \\ &= \sum_{k=0}^{\infty}\frac{(3/2)_k}{2^k k!}g_k(w)z^k\left(\sum_{m=0}^{\infty}\frac{\left(\frac{k}{2}+\frac{3}{4}\right)_m\left(\frac{k}{2}+\frac{5}{4}\right)_m}{m!(k+2)_m}(-z^2)^m\right) \\ &= \sum_{k=0}^{\infty}\frac{(3/2)_k}{2^k k!}g_k(w)z^k\,{}_2F_1\left(\frac{k}{2}+\frac{3}{4},\frac{k}{2}+\frac{5}{4};k+2;-z^2\right),\end{aligned}$$

as claimed. ■

We are ready to prove (4.6). The calculation parallels that in the proofs of Theorems 2.1 and 3.1. Namely, start by estimating in a fairly simple-minded way that

$$\begin{aligned}(4.17)\quad &\left|\varXi(t)-\sum_{n=0}^{N}(-1)^{2n}d_{2n}g_{2n}\left(\frac{t}{2}\right)\right| = \left|\varXi(t)-\sum_{n=0}^{2N}i^n d_n g_n\left(\frac{t}{2}\right)\right| \\ &= \left|\int_0^{\infty}\omega(x)\left[x^{-3/4+it/2}-\sum_{n=0}^{2N}i^n\frac{(3/2)_n}{2^{n-3/2}n!}\,\frac{1}{(x+1)^{3/2}}\left(\frac{x-1}{x+1}\right)^n\right.\right. \\ &\qquad \left.\left.\times\ {}_2F_1\left(\frac{n}{2}+\frac{3}{4},\frac{n}{2}+\frac{5}{4};n+2;\left(\frac{x-1}{x+1}\right)^2\right)g_n\left(\frac{t}{2}\right)\right]dx\right|\end{aligned}$$

$$\le \int_0^\infty \omega(x) \bigg| x^{-3/4+it/2} - \sum_{n=0}^{2N} i^n \frac{(3/2)_n}{2^{n-3/2} n!} \frac{1}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^n$$
$$\times {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right) g_n\left(\frac{t}{2}\right)\bigg|\, dx.$$

By (3.12) and Lemma 4.7 (with $z = i(x-1)/(x+1)$), the kernel $x^{-3/4+it/2}$ can be expanded as

$$x^{-3/4+it/2} = \sum_{n=0}^\infty i^n \frac{(3/2)_n}{2^{n-3/2} n!} \frac{1}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^n$$
$$\times {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right) g_n\left(\frac{t}{2}\right).$$

Continuing the chain of inequalities (4.17), we therefore get

$$\bigg|\Xi(t) - \sum_{n=0}^N (-1)^{2n} d_{2n} g_{2n}\bigg| \le \int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}} \bigg| \sum_{n=2N+1}^\infty i^n \frac{(3/2)_n}{2^{n-3/2} n!} \left(\frac{x-1}{x+1}\right)^n$$
$$\times {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right) g_n(t/2)\bigg|\, dx$$
$$\le \int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}} \sum_{n=2N+1}^\infty \frac{(3/2)_n}{2^{n-3/2} n!} \left|\frac{x-1}{x+1}\right|^n$$
$$\times \left| {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right)\right| \cdot \left| g_n\left(\frac{t}{2}\right)\right| dx$$
$$= \sum_{n=2N+1}^\infty \frac{(3/2)_n}{2^{n-3/2} n!} \left| g_n\left(\frac{t}{2}\right)\right| \int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}} \left|\frac{x-1}{x+1}\right|^n$$
$$\times \left| {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right)\right| dx.$$

Appealing to (4.10) (with a fixed compact set K over which we are allowing t to range) and finally to (4.11), we see that the last expression is bounded by

$$\sum_{n=2N+1}^\infty \frac{(3/2)_n}{2^{n-3/2} n!} C_1 e^{C_2 n^{1/3}} \int_0^\infty \frac{\omega(x)}{(x+1)^{3/2}} \left|\frac{x-1}{x+1}\right|^n$$
$$\times \left| {}_2F_1\left(\frac{n}{2}+\frac{3}{4}, \frac{n}{2}+\frac{5}{4}; n+2; \left(\frac{x-1}{x+1}\right)^2\right)\right| dx$$
$$\le \sum_{n=2N+1}^\infty \frac{(3/2)_n}{2^{n-3/2} n!} C_1 e^{C_2 n^{1/3}} \times J_1 e^{-J_2 n^{2/3}} = O(e^{-\frac{J_2}{2} n^{2/3}})$$

as $n \to \infty$; this gives (4.6) and finishes the proof of Theorem 4.2. ∎

4.3. Asymptotic analysis of the coefficients d_{2n}. In this section we prove Theorem 4.3. We will give two independent proofs of this result, one relying on the representation (4.4) of the coefficients d_{2n} in terms of the coefficients c_{2k}—whose asymptotic behavior we already analyzed—and another relying on a separate representation of d_{2n} as a double integral, which seems of independent interest.

First proof of Theorem 4.3. Our starting point is the formula (4.4). We begin by rewriting this relation in a form that is slightly more convenient for asymptotics,

$$\begin{aligned} d_{2n} &= \frac{2n+1}{2^{2n}} \sum_{m=0}^{\infty} \frac{(3/2)_{2n+2m}}{2^{2m} m!(2n+m+1)!} c_{2n+2m} \\ &= \frac{2n+1}{2^{2n}} \sum_{m=0}^{\infty} \frac{(4n+4m+2)!}{2^{4n+6m+1} m!(2n+m+1)!(2n+2m+1)!} c_{2n+2m} \\ &= \frac{1}{2}(2n+1) \sum_{k=n}^{\infty} \frac{1}{2^{6k}} \frac{(4k+2)!}{(k-n)!(k+n+1)!(2k+1)!} c_{2k}, \end{aligned}$$

substituting $k = n+m$ in the last step. Making use of (3.6), we get

$$\begin{aligned} d_{2n} &= (1+O(n^{-1/10}))128\sqrt{2}\,\pi^{3/2} n \\ &\quad \times \sum_{k=n}^{\infty} \frac{k^{3/2}}{k+n} \cdot \frac{(4k)!}{2^{6k}(k-n)!(k+n)!(2k)!} e^{-4\sqrt{\pi k}} \\ &= (1+O(n^{-1/10}))128\sqrt{2}\,\pi^{3/2} n \\ &\quad \times \sum_{k=n}^{\infty} \frac{k^{3/2}}{k+n} \cdot \frac{1}{2^{4k}} \binom{4k}{2k} \times \frac{1}{2^{2k}} \binom{2k}{k-n} e^{-4\sqrt{\pi k}}, \end{aligned}$$

where for convenience the terms have been simplified slightly by making use of trivial approximations such as $4k+2 = (1+O(n^{-1}))4k$, etc.; the errors in these approximations are absorbed into the leading $1+O(n^{-1/10})$ factor. By Stirling's approximation, the binomial coefficients in the summand have asymptotic behavior

$$\begin{aligned} \frac{1}{2^{4k}} \binom{4k}{2k} &= (1+O(n^{-1})) \frac{1}{\sqrt{2\pi k}} && (k \geq n,\ n \to \infty), \\ \frac{1}{2^{2k}} \binom{2k}{k-n} &= \left(1 + O\left(\frac{1}{k-n}\right)\right) \frac{\sqrt{k}}{\sqrt{\pi(k-n)(k+n)}} \\ &\quad \times \left(\left(\frac{k-n}{k}\right)^{-(k-n)} \left(\frac{k+n}{k}\right)^{-(k+n)} \right) && (k \geq n,\ n \to \infty), \end{aligned}$$

Here, the error term $1 + O(k-n)^{-1}$ is slightly bothersome as it makes it necessary to separately bound the summands for the values of k near n, but this is easy enough to do: observe that if $n \le k \le 2n$ then $k - n \le k/2$, and in this case we find for some constant $C > 0$ independent of n that

$$\binom{2k}{k-n} \le \binom{2k}{\lceil k/2 \rceil} \le C(1.8)^{2k},$$

using Stirling's formula or a well-known bound such as [3, p. 113, eq. (4.7.1)]. Thus, combining the latest estimates, we obtain the expression

$$\begin{aligned} d_{2n} &= (1 + O(n^{-1/10})) \cdot 128\sqrt{\pi}\, n \\ &\quad \times \Bigg[\sum_{k=2n}^{\infty} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \\ &\quad \times \left(\left(\frac{k-n}{k}\right)^{-(k-n)} \left(\frac{k+n}{k}\right)^{-(k+n)} \right) e^{-4\sqrt{\pi k}} + O((0.9)^{2n}) \Bigg] \\ &= (1 + O(n^{-1/10})) \cdot 128\sqrt{\pi}\, n \\ &\quad \times \sum_{k=2n}^{\infty} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \exp\left(n^{2/3} \phi_n\left(\frac{k}{n^{4/3}}\right)\right), \end{aligned} \tag{4.18}$$

where we denote

$$\phi_n(t) = \frac{-(n^{4/3}t - n)\log\left(1 - \frac{n^{-1/3}}{t}\right) - (n^{4/3}t + n)\log\left(1 + \frac{n^{-1/3}}{t}\right)}{n^{2/3}} - 4\sqrt{\pi t}.$$

We are now in a position to apply what is essentially a variant of Laplace's method in the setting of a discrete sum. The following claims about the functions $\phi_n(t)$ are clearly relevant.

LEMMA 4.8.

(i) *We have*

$$\phi_n(t) \le F(t) := -\frac{1}{t} - 4\sqrt{\pi t} \tag{4.19}$$

for all $n \ge 1$ and $t \ge 2n^{-1/3}$.

(ii) *For $1/10 \le t \le 10$ we have the asymptotic relation*

$$\phi_n(t) = F(t) - \frac{1}{6t^3} n^{-2/3} + O\left(\frac{1}{n^{4/3}}\right) \quad \text{as } n \to \infty, \tag{4.20}$$

where the constant implicit in the big-O is independent of n and t, subject to the specified constraint.

Proof. Consider the function of a real variable $0 < x < 1$ given by

$$p(x) = -\left(\frac{1}{x} - 1\right)\log(1-x) - \left(\frac{1}{x} + 1\right)\log(1+x).$$

It is easy to verify that $p(x)$ has the Taylor expansion

$$p(x) = -x - \frac{x^3}{6} - \frac{x^5}{3\times 5} - \frac{x^7}{4\times 7} - \frac{x^9}{5\times 9} - \cdots = -\sum_{m=1}^{\infty} \frac{x^{2m-1}}{m(2m-1)}.$$

In particular, $p(x) \le -x$ for all $0 \le x < 1$. Substituting $x = 1/(n^{1/3}t)$ gives the first claim of the lemma, and the second claim is obtained from the same substitution applied to the fact that $p(x) = -x - \frac{1}{6}x^3 + O(x^5)$ for $0 \le x \le 1/2$. ∎

Some additional easy facts to note are that the function $F(t)$ has a unique global maximum at $t = \alpha_0 := (4\pi)^{-1/3}$; that $F(t)$ is increasing on $(0, \alpha_0)$ and decreasing on (α_0, ∞); that $F(\alpha_0) = -E$ (where E is defined in (4.8)); and that $F''(\alpha_0) = -6\pi$. In particular, we have the Taylor expansion

$$F(t) = -E - 3\pi(t-\alpha_0)^2 + O(|t-\alpha_0|^3) \qquad (1/10 \le t \le 10). \tag{4.21}$$

Now, split up the sum in (4.18) (without the leading numerical constant) into four parts, representing it as $S_n^{(1)} + S_n^{(2)} + S_n^{(3)} + S_n^{(4)}$, where

$$S_n^{(1)} = \sum_{k\,:\,2n\le k<\alpha_0 n^{4/3}-n^{19/18}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \exp\left(n^{2/3}\phi_n\left(\frac{k}{n^{4/3}}\right)\right),$$

$$S_n^{(2)} = \sum_{k\,:\,|k-\alpha_0 n^{4/3}|\le n^{19/18}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \exp\left(n^{2/3}\phi_n\left(\frac{k}{n^{4/3}}\right)\right),$$

$$S_n^{(3)} = \sum_{k\,:\,\alpha_0 n^{4/3}+n^{19/18}<k\le 2n^{4/3}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \exp\left(n^{2/3}\phi_n\left(\frac{k}{n^{4/3}}\right)\right),$$

$$S_n^{(4)} = \sum_{k\,:\,k>2n^{4/3}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \exp\left(n^{2/3}\phi_n\left(\frac{k}{n^{4/3}}\right)\right).$$

Of these four sums, it is $S_n^{(2)}$ that makes the asymptotically most significant contribution. Making use of (4.20) and (4.21), we can estimate it for large n as

$$\begin{aligned} S_n^{(2)} &= \sum_{|k-\alpha_0 n^{4/3}|\le n^{19/18}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \\ &\qquad\qquad \times \exp\left[n^{2/3}\left(F\left(\frac{k}{n^{4/3}}\right) - \frac{n^{10/3}}{6k^3} + O(n^{-4/3})\right)\right] \\ &= (1+O(n^{-2/3})) \sum_{|k-\alpha_0 n^{4/3}|\le n^{19/18}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \\ &\qquad\qquad \times \exp\left[n^{2/3}F\left(\frac{k}{n^{4/3}}\right) - \frac{1}{6}\alpha_0^{-3}(1+O(n^{-5/18}))\right] \end{aligned}$$

$$= (1+O(n^{-5/18}))e^{-2\pi/3}$$
$$\times \sum_{|k-\alpha_0 n^{4/3}|\le n^{19/18}} \frac{k^{3/2}}{(k+n)^{3/2}(k-n)^{1/2}} \exp\left(n^{2/3}F\left(\frac{k}{n^{4/3}}\right)\right)$$
$$= (1+O(n^{-5/18}))e^{-2\pi/3}(\alpha_0 n^{4/3})^{-1/2}$$
$$\times \sum_{|k-\alpha_0 n^{4/3}|\le n^{19/18}} \exp\left(-En^{2/3} - 3\pi n^{2/3}\left(\frac{k}{n^{4/3}}-\alpha_0\right)^2 + O(n^{-1/6})\right)$$
$$= (1+O(n^{-1/6}))e^{-En^{2/3}-2\pi/3}\alpha_0^{-1/2}n^{-2/3}$$
$$\times \sum_{|k-\alpha_0 n^{4/3}|\le n^{19/18}} \exp\left(-3\pi\left(\frac{k-\alpha_0 n^{4/3}}{n}\right)^2\right).$$

The sum in this last expression can be regarded in the usual way as a Riemann sum for a Gaussian integral; specifically, it is asymptotically equal to

$$(1+O(n^{-1}))n\int_{-n^{1/18}}^{n^{1/18}} e^{-3\pi u^2}\,du = (1+O(n^{-1}))n\left(\frac{1}{\sqrt{3}} - O(e^{-n^{1/9}})\right)$$
$$= (1+O(n^{-1}))\frac{n}{\sqrt{3}}$$

as $n\to\infty$ (again making use of (2.39) to justify the first transition). Thus, we have obtained the relation

$$S_n^{(2)} = (1+O(n^{-1/6}))\frac{\alpha_0^{-1/2}}{\sqrt{3}}n^{1/3}e^{-En^{2/3}-2\pi/3} \qquad (n\to\infty).$$

Next, we bound the sum $S_n^{(1)}$ to show that its contribution is negligible compared to that of $S_n^{(2)}$. The polynomial-order factor appearing in front of the exponential term in the sum is bounded from above by 1. Thus, by (4.19) and the fact that $F(t)$ is increasing on $(0,\alpha_0)$, we see that, as $n\to\infty$,

$$0 \le S_n^{(1)} \le \sum_{2n\le k<\alpha_0 n^{4/3}-n^{19/18}} \exp\left(n^{2/3}\phi_n\left(\frac{k}{n^{4/3}}\right)\right)$$
$$\le \sum_{2n\le k<\alpha_0 n^{4/3}-n^{19/18}} \exp\left(n^{2/3}F\left(\frac{k}{n^{4/3}}\right)\right)$$
$$\le \alpha_0 n^{4/3}\exp(n^{2/3}F(\alpha_0 - n^{-5/18}))$$
$$\le \alpha_0 n^{4/3}\exp(-En^{2/3} - 3\pi n^{1/9} + O(n^{-1/6})) = O(e^{-En^{2/3}-n^{1/9}}).$$

The third sum $S_n^{(3)}$ can be bounded in a completely analogous fashion, resulting (the reader can easily check) in the same bound

$$S_n^{(3)} = O(e^{-En^{2/3}-n^{1/9}}).$$

Finally, to bound $S_n^{(4)}$, we use the fact that $F(t) \le -4\sqrt{\pi t}$ to write

$$
\begin{aligned}
0 \le S_n^{(4)} &\le \sum_{k>2n^{4/3}} \frac{10}{k^{1/2}} \exp\left(n^{2/3} F\left(\frac{k}{n^{4/3}}\right)\right) \le \sum_{k>2n^{4/3}} \frac{10}{k^{1/2}} \exp(-4\sqrt{\pi k}) \\
&\le 10 \int_{2n^{4/3}}^{\infty} e^{-4\sqrt{\pi x}}\, dx = \frac{10}{8\pi}(4\sqrt{2\pi}\, n^{2/3} + 1) \exp(-4\sqrt{2\pi}\, n^{2/3}) \\
&= O(e^{-En^{2/3} - n^{1/9}}).
\end{aligned}
$$

Combining the above estimates for $S_n^{(1)}$, $S_n^{(2)}$, $S_n^{(3)}$ and $S_n^{(4)}$, we deduce finally from (4.18) that

$$
d_{2n} = (1 + O(n^{-1/10}))(128\sqrt{\pi}\, n)\left(\frac{\alpha_0^{-1/2}}{\sqrt{3}} n^{1/3} e^{-En^{2/3} - 2\pi/3}\right) \quad \text{as } n \to \infty,
$$

which, after a trivial reshuffling of the terms, is exactly (4.7). Thus, Theorem 4.3 is proved. ∎

Second method for proving Theorem 4.3. We give most of the details of a second proof of Theorem 4.3, except for the rate of convergence result, which we weaken to a less explicit $1 + o(1)$ multiplicative error term. This seems of independent interest as it highlights yet another way of approaching the study of the coefficients d_{2n}. This proof requires some calculations that would be tedious to perform by hand, but are easily done using a computer algebra system (we used Mathematica). We omit the details of these calculations and a few other details needed to make the proof watertight; they may be filled in by an enthusiastic reader.

We start by deriving a new representation of d_{2n} suitable for asymptotic analysis. Begin with the formula (4.1) for d_{2n} in a slightly modified form:

$$
\begin{aligned}
d_{2n} = \frac{(3/2)_{2n}}{2^{2n-5/2}(2n)!} \int_1^{\infty} \frac{\omega(x)}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^{2n} & \\
\times {}_2F_1\left(n + \frac{3}{4}, n + \frac{5}{4}; 2n+2; \left(\frac{x-1}{x+1}\right)^2\right) dx &
\end{aligned}
$$

in which the integration is performed on $(1, \infty)$ (this follows from (4.1) by the same symmetry under the change of variables $u = 1/x$ as in (3.2), a consequence of the functional equation (1.9)). Now use Euler's integral representation

$$
{}_2F_1(a, b; c; z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 t^{b-1}(1-t)^{c-b-1} \frac{1}{(1-zt)^a}\, dt
$$

for the Gauss hypergeometric function (see [1, p. 65]) to represent the ${}_2F_1$ term inside the integral. This gives

$$d_{2n} = \frac{(3/2)_{2n}}{2^{2n-5/2}(2n)!} \frac{\Gamma(2n+2)}{\Gamma(n+3/4)\Gamma(n+5/4)} \times \int_1^\infty \int_0^1 \frac{\omega(x)}{(x+1)^{3/2}} \left(\frac{x-1}{x+1}\right)^{2n} t^{n+1/4}(1-t)^{n-1/4} \times \left(1 - \left(\frac{x-1}{x+1}\right)^2 t\right)^{-(n+3/4)} dt\,dx.$$

As the reader can check, the constant in front of the integral simplifies to

$$\frac{(2n+1)(3/2)_{2n}}{2^{2n-5/2}\Gamma(n+3/4)\Gamma(n+5/4)} = \frac{16}{\pi}(2n+1).$$

Thus, after some further trivial algebraic manipulations we arrive at

$$d_{2n} = \frac{16}{\pi}(2n+1) \int_1^\infty \int_0^1 \frac{\omega(x)}{((x+1)^2 - t(x-1)^2)^{3/4}} \left(\frac{t}{1-t}\right)^{1/4} \times \left(\frac{t(1-t)(x-1)^2}{(x+1)^2 - t(x-1)^2}\right)^n dt\,dx. \tag{4.22}$$

Recalling (2.7), we see that it makes sense to write

$$d_{2n} = \frac{16}{\pi}(2n+1)(R_n + \mu_n), \tag{4.23}$$

where we define the quantities R_n, μ_n by

$$R_n = \int_1^\infty \int_0^1 \frac{\pi x(2\pi x - 3)}{((x+1)^2 - t(x-1)^2)^{3/4}} \left(\frac{t}{1-t}\right)^{1/4} \times e^{-\pi x} \left(\frac{t(1-t)(x-1)^2}{(x+1)^2 - t(x-1)^2}\right)^n dt\,dx, \tag{4.24}$$

$$\mu_n = \int_1^\infty \int_0^1 \frac{\omega(x) - \pi x(2\pi x - 3)e^{-\pi x}}{((x+1)^2 - t(x-1)^2)^{3/4}} \left(\frac{t}{1-t}\right)^{1/4} \times \left(\frac{t(1-t)(x-1)^2}{(x+1)^2 - t(x-1)^2}\right)^n dt\,dx. \tag{4.25}$$

It will be enough to obtain the asymptotic behavior of R_n as $n \to \infty$, and separately to show that μ_n is asymptotically negligible compared to R_n.

PART 1: *Deriving asymptotics for R_n.* Define functions

$$g(t,x) = \frac{\pi x(2\pi x - 3)}{((x+1)^2 - t(x-1)^2)^{3/4}} \left(\frac{t}{1-t}\right)^{1/4},$$

$$h_n(t,x) = \frac{n}{\pi} \log\left(\frac{t(1-t)(x-1)^2}{(x+1)^2 - t(x-1)^2}\right) - x = M \log\left(\frac{t(1-t)(x-1)^2}{(x+1)^2 - t(x-1)^2}\right) - x,$$

where for convenience throughout the proof we denote $M = n/\pi$. Then R_n can be rewritten in the form

$$R_n = \int_1^\infty \int_0^1 g(t,x) \exp(\pi h_n(t,x))\, dt\, dx. \tag{4.26}$$

This form is suitable for applying a two-dimensional version of Laplace's method. The method consists of identifying the global minimum point of $h_n(\cdot,\cdot)$ and analyzing the second-order Taylor expansion of h_n around the minimum point. We will need the partial derivatives of $h_n(\cdot,\cdot)$ up to second order, which after some calculation are found to be

$$\frac{\partial h_n}{\partial x} = \frac{4M(x+1) - (x-1)((x+1)^2 - t(x-1)^2)}{(x-1)((x+1)^2 - t(x-1)^2)}, \tag{4.27}$$

$$\frac{\partial h_n}{\partial t} = -M \frac{(2t-1)(x+1)^2 - t^2(x-1)^2}{t(1-t)((x+1)^2 - t(x-1)^2}, \tag{4.28}$$

$$\frac{\partial^2 h_n}{\partial t^2} = -M \frac{t^4(x-1)^4 + (x+1)^4 - 4t^3(x^2-1)^2 - 4t(x+1)^2(x^2+1) + 2t^2(x+1)^2(3x^2-2x+3)}{t^2(1-t)^2((x+1)^2 - t(x-1)^2)^2}, \tag{4.29}$$

$$\frac{\partial^2 h_n}{\partial x^2} = -8M \frac{x(x+1)^2 - t(x^3 - 3x + 2)}{(x-1)^2((x+1)^2 - t(x-1)^2)}, \tag{4.30}$$

$$\frac{\partial^2 h_n}{\partial t \partial x} = 4M \frac{x^2 - 1}{((x+1)^2 - t(x-1)^2)^2}. \tag{4.31}$$

To find the minimum point, we solve the equations $\frac{\partial h_n}{\partial t} = \frac{\partial h_n}{\partial t} = 0$. By the formulas (4.27)–(4.28), this gives the system of two equations

$$4M(x+1) - (x-1)((x+1)^2 - t(x-1)^2) = 0, \tag{4.32}$$

$$(2t-1)(x+1)^2 - t^2(x-1)^2 = 0. \tag{4.33}$$

Solving (4.32) (a linear equation in t) for t gives the relation

$$t = \frac{(x+1)(x^2 - 4M - 1)}{(x-1)^3}. \tag{4.34}$$

Substituting this value back into (4.33) gives the equation

$$\frac{4(x+1)^2}{(x-1)^4}(x(x-1)^2 - 4M^2) = 0.$$

That is, x has to satisfy the cubic equation

$$x(x-1)^2 - 4M^2 = 0.$$

For $M \geq 1$, one can check that the cubic has a single real solution, given by

$$x = \frac{((54M^2 - 1 + 6M\sqrt{3(27M^2-1)})^{1/3} + 1)^2}{3(54M^2 - 1 + 6M\sqrt{3(27M^2-1)})^{1/3}}. \tag{4.35}$$

The corresponding t-value is given by (4.34), which, for x given by (4.35), can be brought to the slightly simpler form

$$t = \frac{1}{2M^3}[(2M-1)x^2 + (-2M^2+1)x + 2M^2(M-2)].$$

Summarizing the above remarks, define quantities

$$\alpha_n = 54M^2 - 1 + 6M\sqrt{3(27M^2-1)}, \tag{4.36}$$

$$\xi_n = \frac{(\alpha_n^{1/3}+1)^2}{3\alpha_n^{1/3}}, \tag{4.37}$$

$$\tau_n = \frac{1}{2M^3}\big((2M-1)\xi_n^2 + (-2M^2+1)\xi_n + 2M^2(M-2)\big). \tag{4.38}$$

Then (τ_n, ξ_n) is the unique solution of the equations

$$\frac{\partial h_n}{\partial x}(\tau_n,\xi_n) = 0,$$
$$\frac{\partial h_n}{\partial t}(\tau_n,\xi_n) = 0.$$

Using these formulas one can now also find the asymptotic behavior of ξ_n and τ_n as $M \to \infty$, which is given by

$$\tau_n = 1 - 2^{2/3}M^{-1/3} + 2^{4/3}M^{-2/3} - \frac{8}{3}M^{-1} + O(M^{-4/3}),$$
$$\xi_n = 2^{2/3}M^{2/3} + \frac{2}{3} + \frac{1}{9\times 2^{2/3}}M^{-2/3} + O(M^{-4/3}).$$

In particular, note that for large M (that is, for large n) we have $\xi_n > 1$, $0 < \tau_n < 1$. That is, the point (ξ_n, τ_n) lies in the (interior of) the region of integration in the expression (4.26) for R_n.

Next, having found the values (τ_n, ξ_n), we want to understand the values $h_n(\tau_n,\xi_n)$, $\frac{\partial^2 h_n}{\partial t^2}(\tau_n,\xi_n)$, $\frac{\partial^2 h_n}{\partial x^2}(\tau_n,\xi_n)$, $\frac{\partial^2 h_n}{\partial t\partial x}(\tau_n,\xi_n)$. These are somewhat complicated numbers, but can be brought to simpler forms by taking the relevant rational functions in τ_n, ξ_n, expressing them as rational functions of ξ_n only using (4.34), and then performing polynomial reduction modulo the polynomial $\xi_n(\xi_n-1)^2 - 4M^2$ (the cubic polynomial of which ξ_n is a root). Using Mathematica to perform the reduction, we arrived at the following simplified formulas:

$$\frac{\tau_n(1-\tau_n)(\xi_n-1)^2}{(\xi_n+1)^2 - \tau_n(\xi_n-1)^2} = \frac{1}{M^3}\big[(2M-1)\xi_n^2 + (-2M^2+1)\xi_n + M^2(M-4)\big] = 2\tau_n - 1,$$

$$h_n(\tau_n,\xi_n) = M\log\left(\frac{\tau_n(1-\tau_n)(\xi_n-1)^2}{(\xi_n+1)^2-\tau_n(\xi_n-1)^2}\right) - \xi_n = -M\log(2\tau_n-1) - \xi_n,$$

$$\frac{\partial^2 h_n}{\partial t^2}(\tau_n,\xi_n) = -\frac{1}{2(M^2+1)}\big[(M^2+3)\xi_n^2 + 2(2M^2-1)\xi_n + (8M^3-9M^2+8M-1)\big],$$

$$\frac{\partial^2 h_n}{\partial x^2}(\tau_n,\xi_n) = -\frac{1}{4M^2(M^2+1)}\big((2M^2+3)\xi_n^2 - 3\xi_n - 4M(M^2+M+1)\big),$$

$$\frac{\partial^2 h_n}{\partial t\partial x}(\tau_n,\xi_n) = \frac{1}{4M(M^2+1)}\big((M^2-1)\xi_n^2 - 2(2M^2-1)\xi_n + (7M^2-1)\big).$$

Finally, the Hessian

$$\Delta_n := \frac{\partial^2 h_n}{\partial t^2}(\tau_n,\xi_n)\frac{\partial^2 h_n}{\partial x^2}(\tau_n,\xi_n) - \left(\frac{\partial^2 h_n}{\partial t\partial x}(\tau_n,\xi_n)\right)^2$$

can be found to be expressible by the (still ungainly) formula

$$\Delta_n = \frac{(24M^3-17M^2+24M-1)\xi_n^2+2(6M^4-16M^3+31M^2-16M+1)+(56M^4+8M^3-9M^2+8M-1)}{16M^2(M^2+1)}.$$

From these expressions and (4.37), we derive some additional useful asymptotic expansions:

$$\frac{\partial^2 h_n}{\partial x^2}(\tau_n,\xi_n) = -2^{1/3}M^{-2/3} + O(M^{-1}), \tag{4.39}$$

$$\Delta_n = \frac{3}{2^{4/3}}M^{2/3} + O(M^{-1/3}), \tag{4.40}$$

$$\frac{1}{\sqrt{\Delta_n}} = \frac{2^{2/3}}{\sqrt{3}}M^{-1/3} - \frac{2^{4/3}}{\sqrt{3}}M^{-2/3} + \frac{10}{3\sqrt{3}}M^{-1} + O(M^{-4/3}), \tag{4.41}$$

$$h_n(\tau_n,\xi_n) = -3\times 2^{2/3}M^{2/3} - \frac{2}{3} - \frac{1}{15\times 2^{2/3}}M^{-2/3} + O(M^{-4/3}). \tag{4.42}$$

One additional quantity we need to understand is

$$g(\tau_n,\xi_n) = \frac{\pi\xi_n(2\pi\xi_n-3)}{((\xi_n+1)^2-\tau_n(\xi_n-1)^2)^{3/4}}\left(\frac{\tau_n}{1-\tau_n}\right)^{1/4}.$$

This can be written as

$$g(\tau_n,\xi_n) = \pi\xi_n(2\pi\xi_n-3)X_n^{1/4}Y_n^{3/4}$$

where we define

$$X_n = \frac{\tau_n}{1-\tau_n}, \qquad Y_n = \frac{1}{(\xi_n+1)^2-\tau_n(\xi_n-1)^2}.$$

Some more algebraic simplification then shows that

$$X_n = \frac{1}{4M}(\xi_n^2-1), \qquad Y_n = \frac{1}{8M(M^2+1)}(-\xi_n^2+3\xi_n+2(M^2-1)).$$

Using these relations, we then get the asymptotic expansion

$$g(\tau_n,\xi_n) = 2^{2/3}\pi^2 M^{2/3} - \tfrac{1}{6}\pi(9-\pi) + O(M^{-2/3}). \tag{4.43}$$

Now note that (4.39) and (4.40) imply that (for large n) the Hessian matrix of h_n at (τ_n,ξ_n) is negative-definite. Thus, (τ_n,ξ_n) is indeed a local maximum point of h_n. We leave it to the reader to check that it is in fact a *global* maximum.

Now recall that the two-dimensional version of Laplace's method gives the asymptotic formula

$$(1+o(1))\frac{2}{\sqrt{\Delta_n}} g(\tau_n,\xi_n)\exp(\pi h_n(\tau_n,\xi_n))$$

for the integral on the right-hand side of (4.26). This arises by making a suitable change of variables in the integral to center it around the point (ξ_n,τ_n) and introduce scaling that turns the integral into an approximate Gaussian integral—see [70, Ch. VIII] for details; we omit the derivation of bounds needed to rigorously justify the approximation. Substituting the asymptotic values found in (4.41), (4.42) and (4.43) therefore gives

(4.44)

$$\begin{aligned} R_n &= (1+o(1))2\times\left(\frac{2^{2/3}}{\sqrt{3}}M^{-1/3}\right)2^{2/3}\pi^2M^{2/3}\exp\left(-3\times 2^{2/3}\pi M^{2/3} - \frac{2\pi}{3}\right) \\ &= (1+o(1))\left(2\times\frac{2^{2/3}}{\sqrt{3}}\pi^{1/3}\times 2^{2/3}\pi^2\frac{1}{\pi^{2/3}}e^{-2\pi/3}\right)n^{1/3} \\ &\quad\times\exp(-3\times 2^{2/3}\pi^{1/3}n^{2/3}) \\ &= (1+o(1))\left(\frac{4\times 2^{1/3}}{\sqrt{3}}\pi^{5/3}e^{-2\pi/3}\right)n^{1/3}\exp(-3(4\pi)^{1/3}n^{2/3}). \end{aligned}$$

Part 2: *Bounding* μ_n. The next step is to prove that the contribution of μ_n is asymptotically negligible relative to R_n. This relies as usual on (2.7). We sketch the argument but leave the details to the interested reader to develop. Observe that by (2.7), μ_n satisfies a bound of the form

$$\begin{aligned} |\mu_n| &\le C\int_1^\infty\int_0^1 g(t,x)\exp(\pi h_n(t,x)-2\pi x)\,dt\,dx \\ &= C\int_1^\infty\int_0^1 g(t,x)\exp(\pi k_n(t,x))\,dt\,dx \end{aligned}$$

for some constant $C>0$, where we denote $k_n(t,x) = h_n(t,x)-2x$. But now $k_n(t,x)$ can be analyzed in a similar fashion to our analysis of $h_n(t,x)$ above. In particular, it can be shown that for n large enough, $k_n(t,x)$ has a unique global maximum point $(t_n, x_n) \in (0,1)\times(1,\infty)$, and that the maximum value

$$K_n^* := k_n(t_n, x_n)$$

behaves asymptotically as

$$K_n^* = c_0 M^{2/3} + o(M^{2/3})$$

for some constant c_0, where, significantly, $c_0 < -3 \times 2^{2/3}$ (the leading constant in the analogous asymptotic expression (4.42) for the maximum value of $h_n(t,x)$). By deriving some auxiliary technical bounds for the decay of $h_n(t,x)$ away from its maximum point and near the boundaries of the integration region, one can then show that for any $\epsilon > 0$, μ_n satisfies a bound of the form

$$|\mu_n| = O\big(\exp(\pi^{1/3}(c_0+\epsilon)n^{2/3})\big).$$

Taking $\epsilon < 3 \times 2^{2/3} - c_0$ then gives a rate of growth that is smaller than the exponential rate of growth of R_n, establishing that $\mu_n \ll R_n$.

PART 3: *Putting everything together.* Combining the above discussion regarding μ_n with (4.23) and (4.44), we find that

$$\begin{aligned} d_{2n} &= (1+o(1))\left(\frac{16}{\pi}(2n+1)\right) \times \left(\frac{4\times 2^{1/3}}{\sqrt{3}}\pi^{5/3}e^{-2\pi/3}\right)n^{1/3} \\ &\quad \times \exp(-3(4\pi)^{1/3}n^{2/3}) \\ &= (1+o(1))\left(\frac{128\times 2^{1/3}}{\sqrt{3}}\pi^{2/3}e^{-2\pi/3}\right)n^{4/3}\exp(-3(4\pi)^{1/3}n^{2/3}), \end{aligned}$$

which is the same (except for the weaker rate of convergence estimate) as (4.7). ∎

5. An asymptotic formula for the Taylor coefficients of $\Xi(t)$. The method we used in Section 2 to analyze the asymptotic behavior of the Hermite expansion coefficients b_{2n} has the added benefit of enabling us to also prove an analogous asymptotic formula for the Taylor coefficients a_{2n} in the Taylor expansion (1.4) of the Riemann xi function. The reason for this is a pleasing similarity between the formulas for a_{2n} and b_{2n}. It was noted by the authors of [14] and [16] (and probably others before them) that the formula for a_{2n} can be written in the form

$$a_{2n} = \frac{2}{(2n)!}\int_0^\infty \Phi(x)x^{2n}\,dx = \frac{1}{(2n)!}\int_{-\infty}^\infty \Phi(x)x^{2n}\,dx, \tag{5.1}$$

as can be seen by performing the usual change of variables $x = e^{2u}$ in (1.5) (or by differentiating $2n$ times under the integral sign in (1.11) and setting $t = 0$). The striking resemblence of this formula to (1.13) seems however to have gone unremarked in the literature.

THEOREM 5.1 (Asymptotic formula for the coefficients a_{2n}). *The coefficients a_{2n} satisfy the asymptotic formula*

$$(5.2)\qquad a_{2n} = \left(1+O\left(\frac{\log\log n}{\log n}\right)\right)\frac{\pi^{1/4}}{2^{2n-5/2}(2n)!}\left(\frac{2n}{\log(2n)}\right)^{7/4} \times \exp\left[2n\left(\log\left(\frac{2n}{\pi}\right)-W\left(\frac{2n}{\pi}\right)-\frac{1}{W\left(\frac{2n}{\pi}\right)}\right)\right]$$

as $n\to\infty$, where $W(\cdot)$ denotes as in Section 2 the Lambert W-function.

Proof. The idea is to repeat the analysis in the proof of Theorem 2.7, but with the numbers Q_{2n} and r_{2n} in (2.25)–(2.26) being replaced by

$$(5.3)\qquad Q'_n = \int_0^\infty x^{2n}e^{5x/2}\left(e^{2x}-\frac{3}{2\pi}\right)\exp(-\pi e^{2x})\,dx,$$

$$(5.4)\qquad r'_n = \int_0^\infty x^{2n}e^{5x/2}\sum_{m=2}^\infty\left(m^4e^{2x}-\frac{3m^2}{2\pi}\right)\exp(-\pi m^2e^{2x})\,dx,$$

for which, by (1.8) and (5.1), we then have

$$(5.5)\qquad a_{2n} = \frac{8\pi^2}{(2n)!}(Q'_{2n}+r'_{2n}).$$

Note that the only difference from the original definitions of Q_{2n} and r_{2n} is the absence of the factor $e^{-x^2/4}$. Thus, the analysis carries over essentially verbatim to our current case, except that we replace the function $f(x)$ in the reformulated equation (2.28) for Q_n with

$$\varphi(x) = e^{5x/2}\left(e^{2x}-\frac{3}{2\pi}\right),$$

to get the analogous representation

$$(5.6)\qquad Q'_n = \frac{1}{2^{2n}}\int_0^\infty \varphi(x)\exp(\psi_{2n}(2x))\,dx$$

for Q'_n. The effect of this change on the subsequent formulas is that the factor γ_n in (2.31) then also gets replaced by the simpler factor $\gamma'_n=\varphi(x_{2n}/2)$ in the asymptotic formula

$$(5.7)\qquad Q'_n = \left(1+O\left(\frac{1}{n^{1/5}}\right)\right)\frac{\sqrt{\pi}}{2^{2n}\sqrt{2\beta_n}}\gamma'_n e^{\alpha_n}$$

that is the analogue of (2.42)—the factors β_n and α_n (and, importantly, the maximum point value x_{2n} from which they are derived) remain the same.

Now, γ'_n has the asymptotic behavior (the counterpart to (2.34))

$$(5.8)\qquad \gamma'_n = (1+O(e^{-x_{2n}}))\exp\left(\frac{9}{4}x_{2n}\right) = \left(1+O\left(\frac{\log n}{n}\right)\right)\left(\frac{2n}{\pi x_{2n}}\right)^{9/4}$$

as $n \to \infty$. With these facts in mind, it is now a simple matter to go through the calculations and various bounds in the proof of Theorem 2.7 and verify that they remain valid in the current setting (including the bound (2.45) with Q'_n and r'_n replacing Q_n and r_n, respectively), with the final result being that the relation (2.43) is now replaced by

$$Q'_n = \left(1 + O\left(\frac{\log\log n}{\log n}\right)\right) \frac{1}{2^{2n+1/2}} \left(\frac{2n}{\pi x_{2n}}\right)^{7/4} \times \exp\left[2n\left(\log(2n) - \log\pi - x_{2n} - \frac{1}{x_{2n}}\right)\right].$$

Inserting this into (5.5) gives (5.2). ■

It is interesting to compare our formula (5.2) to other asymptotic formulas for the coefficients a_{2n} which have appeared in the literature. At the time we completed the first version of this paper, the strongest result of this type we were aware of was the one due to Coffey [14, Prop. 1]. Coffey's formula is more explicit, since it contains only elementary functions, but is less accurate, since (if expressed in our notation as a formula for a_{2n} rather than in Coffey's logarithmic notation) it has a multiplicative error term of $\exp(O(1)) = \Theta(1)$, compared to our $1 + O\left(\frac{\log n}{n}\right)$.

After we finished the initial version of this paper, we learned of another recent asymptotic formula for the coefficients a_{2n} that was proved by Griffin, Ono, Rolen and Zagier in their paper (written in 2018) [22, Th. 7] (see also equations (1) and (13) there). Griffin et al.'s result is more accurate than our Theorem 5.1, as it gives a full asymptotic expansion for a_{2n} whereby the relative error term can be made smaller than $o(n^{-K})$ for any fixed K by truncating the expansion after sufficiently many terms. Their formula is expressed in terms of an implicitly defined quantity $L(n)$ that solves the equation

$$n = L(\pi e^L + 3/4).$$

This equation (a slightly more exotic variant of our equation for x_{2n} involving Lambert's W-function) arises out of an application of Laplace's method in a manner quite similar to our own analysis. It is interesting to ask whether our approach can be similarly extended to obtain a full asymptotic expansion for a_{2n} that is expressed in terms of the (arguably simpler) quantities $x_{2n} = W\left(\frac{2n}{\pi}\right)$.

6. Final remarks. We conclude with a few open problems and suggestions for future research.

(1) There has been much discussion in the literature of sufficient conditions guaranteeing that a polynomial $p(z)$ has only real zeros based on knowledge of its coefficients in the expansion $p(z) = \sum_{k=0}^{n} \alpha_k \phi_k(z)$, where

$(\phi_k)_{k=0}^{\infty}$ is some given family of orthogonal polynomials. We note Turán's many results in [66, 67, 68], particularly his observation (Lem. II in [68], a result he discovered independently but attributes to an earlier paper by Pólya [48]) that if the zeros of $\sum_{k=0}^{n} a_k z^k$ are all real then that is also the case for the corresponding Hermite expansion $\sum_{k=0}^{n} a_k H_k(z)$; and the many analogous theorems of Iserles and Saff [28], among them the result (a special case of Prop. 6 in their paper) that if the zeros of the polynomial $\sum_{k=0}^{n} a_k z^k$ are all real then this is also the case for the polynomial $\sum_{k=0}^{n} \frac{k!}{(3/2)_k} a_k f_k(z)$. See also [7, 8, 25, 26, 27, 47] and the survey [61] for further developments along these lines.

One question that now arises naturally is: to what extent do these developments inform the attempts to prove the reality of the zeros of the Riemann xi function, in view of our new results?

(2) One rather striking fact is that the four different series expansions we have considered for the Riemann xi function, namely

$$\varXi(t) = \sum_{n=0}^{\infty} (-1)^n a_{2n} t^{2n}, \qquad \varXi(t) = \sum_{n=0}^{\infty} (-1)^n c_{2n} f_{2n}(t),$$
$$\varXi(t) = \sum_{n=0}^{\infty} (-1)^n b_{2n} H_{2n}(t), \quad \varXi(t) = \sum_{n=0}^{\infty} (-1)^n d_{2n} g_{2n}(t),$$

exhibit remarkable structural similarities: namely, in all four expansions the coefficients appear with alternating signs (and their asymptotics can be understood to a good level of accuracy, as our analysis shows).

It is intriguing to wonder about the significance of this structural property of $\varXi(t)$. Can this information be exploited somehow to derive information about the location of the zeros of $\varXi(t)$?

By way of comparison, one can consider "toy" expansions of the above forms involving more elementary coefficient sequences. For example, we have the trivial expansions (the latter two of which being easy consequences of (A.5) and (A.15), respectively)

$$\sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n}}{(2n)!} t^{2n} = \cos(\alpha t) \qquad (\alpha > 0),$$
$$\sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n}}{(2n)!} H_{2n}(t) = e^{\alpha^2} \cos(2\alpha t) \qquad (\alpha > 0),$$
$$\sum_{n=0}^{\infty} (-1)^n \alpha^{2n} f_{2n}(t) = \frac{2}{(1-\alpha^2)^{3/4}} \cos\left(t \log\left(\frac{1+\alpha}{1-\alpha} \right) \right) \qquad (0 < \alpha < 1),$$

which are entire functions of t that—needless to say—all have only real zeros. On the other hand, we do not know for which values of $\alpha \in (0, 1)$ the expansion (whose explicit form is evaluated using (A.24))

$$\sum_{n=0}^{\infty}(-1)^n\alpha^{2n}g_{2n}(t) = \frac{1}{(1-\alpha)^2}\,{}_2F_1\left(1,\frac{3}{4}-it;\frac{3}{2};\frac{-4\alpha}{(1-\alpha)^2}\right) + \frac{1}{(1+\alpha)^2}\,{}_2F_1\left(1,\frac{3}{4}-it;\frac{3}{2};\frac{4\alpha}{(1+\alpha)^2}\right)$$

has only real zeros.

(3) The notion of Poisson flows we introduced seems worth exploring further. The Poisson flow associated with the polynomial family $(f_n)_{n=0}^{\infty}$ has interesting properties, and while it does not preserve hyperbolicity in the sense of "continuous time" as we discussed in Section 3.5, it seems not inconceivable that a weaker form of preservation of reality of the zeros for discrete time parameter values might still hold. For example, does there exist a constant $0 < r_0 < 1$ such that if the polynomial $\sum_{k=0}^{n} a_k r_0^k f_k(t)$ has only real zeros then the same is guaranteed to be true for the polynomial $\sum_{k=0}^{n} a_k f_k(t)$? It appears like it may be possible to approach this question using the biorthogonality techniques developed in the papers by Iserles and coauthors [25, 26, 27, 28]. And what can be said about the Poisson flow associated with the orthogonal polynomial family $(g_n)_{n=0}^{\infty}$?

Appendix: Orthogonal polynomials. In this Appendix we summarize some background facts we need on the families of orthogonal polynomials discussed in the paper, and prove a few additional auxiliary results. We assume the reader is familiar with the basic theory of orthogonal polynomials, as described, e.g., in Chapters 2–3 of Szegő's classical book [63].

A.1. Hermite polynomials. The Hermite polynomials are the well-known sequence $H_n(x)$ of polynomials that are orthogonal with respect to the Gaussian weight function e^{-x^2} on $\mathbb{R}$. A few of their main properties are given below; see [1, Sec. 6.1] for proofs.

(1) Definition:

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}(e^{-x^2}). \tag{A.1}$$

(2) Orthogonality relation:

$$\int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}\,dx = 2^n n!\sqrt{\pi}\,\delta_{m,n}. \tag{A.2}$$

(3) Recurrence relation:

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0. \tag{A.3}$$

(4) Differential equation:

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0. \tag{A.4}$$

(5) Generating function:

$$\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} z^n = \exp(2xz - z^2). \tag{A.5}$$

(6) Poisson kernel:

$$\frac{1}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{H_n(x)H_n(y)}{2^n n!} z^n = \frac{1}{\sqrt{\pi}\sqrt{1-z^2}} \exp\left(\frac{2xyz - (x^2+y^2)z^2}{1-z^2}\right). \tag{A.6}$$

(7) Symmetry: $H_n(-x) = (-1)^n H_n(x)$.

A.2. Symmetric Meixner–Pollaczek polynomials $f_n(x) = P_n^{(3/4)}(x; \pi/2)$. The *Meixner–Pollaczek polynomials* are a two-parameter family of orthogonal polynomial sequences $P_n^{(\lambda)}(x; \phi)$. The parameters satisfy $\lambda > 0$, $0 \le \phi < \pi$. In the special case $\phi = \pi/2$, the polynomials are sometimes referred to as the *symmetric Meixner–Pollaczek polynomials* (see [2]). In this paper we make use of the special case $\lambda = 3/4$ of the symmetric case, namely the polynomials, which we denote $f_n(x)$ for simplicity, given by

$$f_n(x) = P_n^{(3/4)}(x; \pi/2). \tag{A.7}$$

The key property of the $f_n(x)$ is that they are an orthonormal family for the weight function $|\Gamma(3/4 + ix)|^2$, $x \in \mathbb{R}$. Additional properties we need are given in the list below. Bibliographic notes and a few more details regarding proofs are given at the end of this section. See also Section A.4 where we prove additional results relating the polynomial family f_n to another family g_n of orthogonal polynomials, discussed in Section A.3.

(1) Definition and explicit formulas:

$$f_n(x) = \frac{(3/2)_n}{n!} i^n \, {}_2F_1\left(-n, \frac{3}{4} + ix; \frac{3}{2}; 2\right) \tag{A.8}$$

$$= (-i)^n \sum_{k=0}^{n} 2^k \binom{n + \frac{1}{2}}{n-k} \binom{-\frac{3}{4} + ix}{k} \tag{A.9}$$

$$= i^n \sum_{k=0}^{n} (-1)^k 2^k \binom{n + \frac{1}{2}}{n-k} \binom{-\frac{1}{4} + ix + k}{k} \tag{A.10}$$

$$= i^n \sum_{k=0}^{n} (-1)^k \binom{-\frac{3}{4} + ix}{k} \binom{-\frac{3}{4} - ix}{n-k}. \tag{A.11}$$

(2) Orthogonality relation:

$$\int_{-\infty}^{\infty} f_m(x) f_n(x) \left| \Gamma\left(\frac{3}{4} + ix\right)\right|^2 dx = \frac{\pi^{3/2}(3/2)_n}{2\sqrt{2}n!}\delta_{m,n}. \tag{A.12}$$

(3) Recurrence relation:

$$(n+1)f_{n+1}(x) - 2xf_n(x) + \left(n + \frac{1}{2}\right) f_{n-1}(x) = 0. \tag{A.13}$$

(4) Difference equation:

$$2\left(n + \frac{3}{4}\right) f_n(x) - \left(\frac{3}{4} - ix\right) f_n(x+i) - \left(\frac{3}{4} + ix\right) f_n(x-i) = 0. \tag{A.14}$$

(5) Generating function:

$$\sum_{n=0}^{\infty} f_n(x) z^n = (1-iz)^{-\frac{3}{4}+ix}(1+iz)^{-\frac{3}{4}-ix} = \frac{1}{(1+z^2)^{\frac{3}{4}}}\left(\frac{1-iz}{1+iz}\right)^{ix}. \tag{A.15}$$

(6) Poisson kernel:

$$\begin{aligned} &\frac{2\sqrt{2}}{\pi^{3/2}} \sum_{n=0}^{\infty} \frac{n!}{(3/2)_n} f_n(x) f_n(y) z^n \\ &= \frac{2\sqrt{2}}{\pi^{3/2}} \frac{1}{(1-z)^{3/2}} \left(\frac{1+z}{1-z}\right)^{i(x+y)} {}_2F_1\left(\frac{3}{4} + ix, \frac{3}{4} + iy; \frac{3}{2}; \frac{-4z}{(1-z)^2}\right). \end{aligned} \tag{A.16}$$

(7) Symmetry: $f_n(-x) = (-1)^n f_n(x)$.

NOTES. The above list is based on the general list of properties of the Meixner–Pollaczek polynomials $P_n^{(\lambda)}(x;\phi)$ provided in [32, pp. 213–216], except for (A.16), which is a special case of [29, eq. (2.25)].

In the formulas (A.8)–(A.11), the first formula is the definition as given in [32]; formula (A.10) is an explicit rewriting of (A.8) as a sum, and (A.9) follows from (A.10) by applying the symmetry property (7) (which in turn is an easy consequence of either the recurrence relation (A.13) or the generating function (A.15)). Formula (A.11) appears to be new, and follows by evaluating the sequence of coefficients of z^n in the generating function (A.15) as a convolution of the coefficient sequences for the functions $(1-iz)^{-3/4+ix}$ and $(1+iz)^{-3/4-ix}$. Note that (A.11) has the benefit of making the odd/even symmetry of $f_n(x)$ readily apparent, which the other explicit formulas do not.

A.3. Continuous Hahn polynomials $g_n(x) = p_n\left(x; \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right)$. The *continuous Hahn polynomials* are a four-parameter family $p_n(x; a, b, c, d)$ of orthogonal polynomial sequences. They were introduced in increasing degrees of generality by Askey and Wilson [4] and later Atakishiyev and Suslov [5] as continuous-weight analogues of the Hahn polynomials; earlier special cases appeared in the work of Bateman [6] and later Pasternack [43] (see also [33] for a chronology of these discoveries and related discussion).

For our purposes, a prominent role will be played by the special case $a = b = c = d = 3/4$ of the continuous Hahn polynomials, that is, the polynomial sequence

$$g_n(x) = p_n\left(x; \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right). \tag{A.17}$$

A few of the main properties of these polynomials we will need are listed below. The notes at the end of the section provide references and additional details.

(1) Definition and explicit formulas:

$$g_n(x) = i^n(n+1)\ {}_3F_2\left(-n, n+2, \frac{3}{4}+ix; \frac{3}{2}, \frac{3}{2}; 1\right) \tag{A.18}$$

$$= (-i)^n \sum_{k=0}^{n} \frac{(n+k+1)!}{(n-k)!(3/2)_k^2} \binom{-\frac{3}{4}+ix}{k} \tag{A.19}$$

$$= i^n \sum_{k=0}^{n} (-1)^k \frac{(n+1)!}{(3/2)_k (3/2)_{n-k}} \binom{-\frac{3}{4}+ix}{k} \binom{-\frac{3}{4}-ix}{n-k}. \tag{A.20}$$

(2) Orthogonality relation:

$$\int_{-\infty}^{\infty} g_m(x) g_n(x) \left| \Gamma\left(\frac{3}{4}+ix\right)\right|^4 dx = \frac{\pi^3}{16}\delta_{m,n}. \tag{A.21}$$

(3) Recurrence relation:

$$(2n+3)g_{n+1}(x) - 8x g_n(x) + (2n+1)g_{n-1}(x) = 0. \tag{A.22}$$

(4) Difference equation:

(A.23)

$$\left((n+1)^2 - 2x^2 + \frac{1}{8}\right) g_n(x) - \left(\frac{3}{4} - ix\right)^2 g_n(x+i) - \left(\frac{3}{4}+ix\right)^2 g_n(x-i) = 0.$$

(5) Generating functions:

$$\sum_{n=0}^{\infty} g_n(x) z^n = \frac{1}{(1+iz)^2}\ {}_2F_1\left(1, \frac{3}{4} - ix; \frac{3}{2}; \frac{4iz}{(1+iz)^2}\right), \tag{A.24}$$

$$\sum_{n=0}^{\infty} \frac{g_n(x)}{(n+1)!} z^n = {}_1F_1\left(\frac{3}{4}+ix; \frac{3}{2}; -iz\right) {}_1F_1\left(\frac{3}{4} - ix; \frac{3}{2}; iz\right). \tag{A.25}$$

(6) Symmetry: $g_n(-x) = (-1)^n g_n(x)$.

Notes. This list is based on the list of properties of the continuous Hahn polynomials $p_n(x; a, b, c, d)$ given in [32, pp. 200–204].

In the formulas (A.18)–(A.20), the first is the definition as given in [32], and (A.19) is the explicit rewriting of (A.18) as a sum. Formula (A.20), which (like (A.11) discussed in the previous section) has the benefit of highlighting the odd/even symmetry of $g_n(x)$, seems new, and is proved by evaluating the coefficient of z^n in (A.25) as

$$\frac{g_n(x)}{(n+1)!} = \sum_{k=0}^{n} [z^k]\left({}_1F_1\left(\frac{3}{4}+ix;\frac{3}{2};-iz\right)\right) \times [z^{n-k}]\left({}_1F_1\left(\frac{3}{4}-ix;\frac{3}{2};iz\right)\right)$$

and simplifying.

A.4. The relationship between the polynomial sequences f_n, g_n. The goal of this section is to prove the following pair of identities, which seem new, relating the two orthogonal polynomial families $(f_n)_{n=0}^\infty$ and $(g_n)_{n=0}^\infty$.

PROPOSITION A.1. *The polynomial families $f_n(x)$ and $g_n(x)$ are related by the equations*

$$g_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{2^{n-2k}(n-k)!}{(3/2)_{n-2k}k!} f_{n-2k}(x), \tag{A.26}$$

$$f_n(x) = \frac{(3/2)_n}{2^n(n+1)!} \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k (n-2k+1)\binom{n+1}{k} g_{n-2k}(x). \tag{A.27}$$

The proofs relies on two binomial summation identities, given in the next two lemmas.

LEMMA A.2. *For integers $p, q \geq 0$ we have the summation identity*

$$\sum_{k=0}^{\lfloor p/2 \rfloor} \frac{(-1)^k (p+q-k)!}{2^{2k} k!(p-2k)!} = \frac{1}{2^p} q! \binom{p+2q+1}{p}. \tag{A.28}$$

Proof. Consider, for fixed $q \geq 0$, the generating function in an indeterminate x of the sequence of numbers (indexed by the parameter $p \geq 0$) on the left-hand side of (A.28). This generating function can be evaluated as

$$\begin{aligned}\sum_{p\geq 0}&\left(\sum_{k=0}^{\lfloor p/2 \rfloor} \frac{(-1)^k (p+q-k)!}{2^{2k} k!(p-2k)!}\right) x^p \\ &= \sum_{p\geq 0}\left(\sum_k \left(-\frac{1}{4}\right)^k \binom{p-k}{k}(p-k+1)\cdots(p-k+q)\right)x^p \\ &= \sum_{m\geq 0}\sum_k \left(-\frac{1}{4}\right)^k \binom{m}{k}(m+1)\cdots(m+q)x^{m+k}\end{aligned}$$

$$= \sum_{m\ge 0}(m+1)\cdots(m+q)x^m\left(\sum_k \binom{m}{k}\left(-\frac{x}{4}\right)^k\right)$$
$$= \sum_{m\ge 0}(m+1)\cdots(m+q)\left(x\left(1-\frac{x}{4}\right)\right)^m = \frac{d^q}{dy^q}\bigg|_{y=x(1-x/4)}\left(\sum_{m=0}^{\infty} y^m\right)$$
$$= \frac{d^q}{dy^q}\bigg|_{y=x(1-x/4)}\left(\frac{1}{1-y}\right) = \frac{q!}{(1-y)^{q+1}}\bigg|_{y=x(1-x/4)}$$
$$= \frac{q!}{(1-x(1-x/4))^{q+1}} = \frac{q!}{(1-x/2)^{2q+2}} = \sum_{p=0}^{\infty}\frac{q!}{2^p}\binom{p+2q+1}{p}x^p,$$

which is the generating function for the sequence on the right-hand side of (A.28). ∎

LEMMA A.3. *We have the summation identity*

$$\sum_{k=0}^{N}(N-2k)\binom{N}{k}\binom{N+m-2k}{2m+1} = N\binom{N-1}{m}2^{N-m} \tag{A.29}$$

for integers $N, m \ge 0$.

Proof. Denote

$$F_m(N,k) = \frac{(N-2k)\binom{N}{k}\binom{N+m-2k}{2m+1}}{N\binom{N-1}{m}2^{N-m}},$$

so that the identity to prove becomes the statement $\sum_{k=0}^{N} F_m(N,k) = 1$. This claim in turn follows by applying the method of Wilf–Zeilberger pairs [46, Ch. 7], [69] to the rational certificate function (in which m is regarded as a parameter)

$$R_m(N,k) = \frac{k(m+N+1-2k)(m+N+2-2k)}{2(N-2k)(N+1-k)(N-m-2k)}.$$

The certificate was found using the Mathematica package `fastZeil` [44, 45], a software implementation of Zeilberger's algorithm. ∎

Proof of (A.26). An immediate consequence of (A.28) is the identity

$$\sum_{k=0}^{\lfloor (n-m)/2\rfloor}\frac{(-1)^k(n-k)!}{2^{2k}k!(3/2)_{n-2k}}\binom{n-2k+\frac{1}{2}}{n-2k-m} = \frac{(n+m+1)!}{2^{n+m}(n-m)!(3/2)_m^2}, \tag{A.30}$$

which holds for integers $n \ge m \ge 0$—indeed, this relation reduces to (A.28) after a short simplification on taking $p = n-m$, $q = m$ and using the facts that $(3/2)_m = \frac{(2m+2)!}{2^{2m+1}(m+1)!}$ and $\binom{n-2k+1/2}{n-2k-m} = \frac{(3/2)_{n-2k}}{(n-2k-m)!(3/2)_m}$. Now (A.30) is the key to proving (A.26): making use of the explicit formulas (A.9) and

(A.19) for $f_n(x)$ and $g_n(x)$, respectively, we write

$$\sum_{k=0}^{\lfloor n/2 \rfloor} \frac{2^{n-2k}(n-k)!}{(3/2)_{n-2k}k!} f_{n-2k}(x)$$
$$= \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{2^{n-2k}(n-k)!}{(3/2)_{n-2k}k!} \left((-i)^{n-2k} \sum_{m=0}^{n-2k} 2^m \binom{n-2k+\frac{1}{2}}{n-2k-m} \binom{-\frac{3}{4}+ix}{m} \right)$$
$$= (-i)^n \sum_{m=0}^{n} \left(2^m \sum_{k=0}^{\lfloor (n-m)/2 \rfloor} \frac{(-1)^k 2^{n-2k}(n-k)!}{(3/2)_{n-2k}k!} \binom{n-2k+\frac{1}{2}}{n-2k-m} \right) \binom{-\frac{3}{4}+ix}{m}$$
$$= (-i)^n \sum_{m=0}^{n} \frac{(n+m+1)!}{(n-m)!(3/2)_m^2} \binom{-\frac{3}{4}+ix}{m} = g_n(x),$$

getting the result. ∎

Proof of (A.27). Using (A.29), we can deduce the slightly more messy identity
(A.31)
$$\frac{(3/2)_n}{2^n (3/2)_m^2} \sum_{k=0}^{\lfloor (n-m)/2 \rfloor} \frac{(n-2k+1)(n-2k+m+1)!}{k!(n-k+1)!(n-2k-m)!} = 2^m \binom{n+1/2}{n-m},$$

valid for $n \geq m \geq 0$. The way to see this is to first massage the left-hand side of (A.29) a bit by rewriting it as

$$\sum_{k=0}^{N} (N-2k) \binom{N}{k} \binom{N+m-2k}{2m+1} = 2 \sum_{k=0}^{\lfloor N/2 \rfloor} (N-2k) \binom{N}{k} \binom{N+m-2k}{2m+1}$$
$$= 2 \sum_{k=0}^{\lfloor \frac{N-m}{2} \rfloor} (N-2k) \binom{N}{k} \binom{N+m-2k}{2m+1},$$

where the first equality follows from the symmetry of the summand under the relabeling $k \mapsto N-k$, and the second equality follows on noticing that the summands actually vanish for values of k for which $\frac{N-m}{2} < k < \frac{N+m}{2}$. Thus, we obtain another variant of (A.29), namely

$$\text{(A.32)} \qquad \sum_{k=0}^{\lfloor (N-m)/2 \rfloor} (N-2k) \binom{N}{k} \binom{N+m-2k}{2m+1} = N \binom{N-1}{m} 2^{N-m+1}.$$

We leave it to the reader to verify (using similar simple substitutions as in the proof of (A.26) above) that setting $N = n+1$ in this new identity gives a relation that is equivalent to (A.31).

Finally, from (A.31) we can prove the relation (A.27) in an analogous manner to the proof of (A.26), again making use of the expansions (A.9), (A.19) but working in the opposite direction. We have

$$\frac{(3/2)_n}{2^n(n+1)!}\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k(n-2k+1)\binom{n+1}{k}g_{n-2k}(x)$$

$$= \frac{(3/2)_n}{2^n(n+1)!}\sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k(n-2k+1)\binom{n+1}{k}$$

$$\times(-i)^{n-2k}\left(\sum_{m=0}^{n-2k}\frac{(n-2k+m+1)!}{(n-2k-m)!(3/2)_m^2}\binom{-\frac{3}{4}+ix}{m}\right)$$

$$= (-i)^n\sum_{m=0}^{n}\left(\frac{(3/2)_n}{2^n}\sum_{k=0}^{\lfloor (n-m)/2\rfloor}\frac{(n-2k+1)(n-2k+m+1)!}{k!(n-k+1)!(n-2k-m)!(3/2)_m^2}\right)\binom{-\frac{3}{4}+ix}{m}$$

$$= f_n(x),$$

as claimed. ∎

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Abstract (will appear on the journal's web site only)

Pál Turán in the 1950s proposed to use the expansion of the Riemann xi function in the Hermite polynomials as a tool to gain insight into the location of the zeros of the Riemann zeta function. In this paper we follow up and expand on Turán's ideas in several ways by considering infinite series expansions for the Riemann xi function $\Xi(t)$ in three specific families of orthogonal polynomials: (1) the Hermite polynomials; (2) the symmetric Meixner–Pollaczek polynomials $P_n^{(3/4)}(x;\pi/2)$; and (3) the continuous Hahn polynomials $p_n\big(x;\frac{3}{4},\frac{3}{4},\frac{3}{4},\frac{3}{4}\big)$. For each of the three expansions we derive asymptotic formulas for the coefficients and prove additional results. We also apply some of the same techniques to prove a new asymptotic formula for the Taylor coefficients of the Riemann xi function, and uncover a previously unnoticed connection between the Hermite expansion of $\Xi(t)$ and the separate program of research involving the de Bruijn–Newman constant.