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Densities of Short Uniform Random Walks

with an appendix by Don Zagier

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Abstract. We study the densities of uniform random walks in the plane. A special focus is on the case of short walks with three or four steps and, less completely, those with five steps. As one of the main results, we obtain a hypergeometric representation of the density for four steps, which complements the classical elliptic representation in the case of three steps. It appears unrealistic to expect similar results for more than five steps. New results are also presented concerning the moments of uniform random walks and, in particular, their derivatives. Relations with Mahler measures are discussed.

1 Introduction

An n-step uniform random walk is a walk in the plane that starts at the origin and consists of n steps of length 1 each taken into a uniformly random direction. The study of such walks largely originated with Pearson more than a century ago [Pea05b, Pea05a, Pea06] who posed the problem of determining the distribution of the distance from the origin after a certain number of steps. In this paper, we study the (radial) densities p_n of the distance travelled in n steps. This continues research begun in [BNSW11, BSW11], where the focus was on the moments of the distributions

$$W_n(s) := \int_0^n p_n(t) t^s \,\mathrm{d}t.$$

The densities for walks of up to 8 steps are depicted in Figure 1. As established by Lord Rayleigh [Ray05], p_n quickly approaches the probability density $\frac{2x}{n} e^{-x^2/n}$ for large n. This limiting density is superimposed in Figure 1 for $n \geqslant 5$.

Closed forms were only known in the cases $n = 2$ and $n = 3$. The evaluation, for $0 \leqslant x \leqslant 2$,

$$p_2(x) = \frac{2}{\pi\sqrt{4 - x^2}} \tag{1.1}$$

is elementary. On the other hand, the density $p_3(x)$ for $0 \leqslant x \leqslant 3$ can be expressed in terms of elliptic integrals by

$$p_3(x) = \operatorname{Re}\left(\frac{\sqrt{x}}{\pi^2} K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}} \right) \right), \tag{1.2}$$

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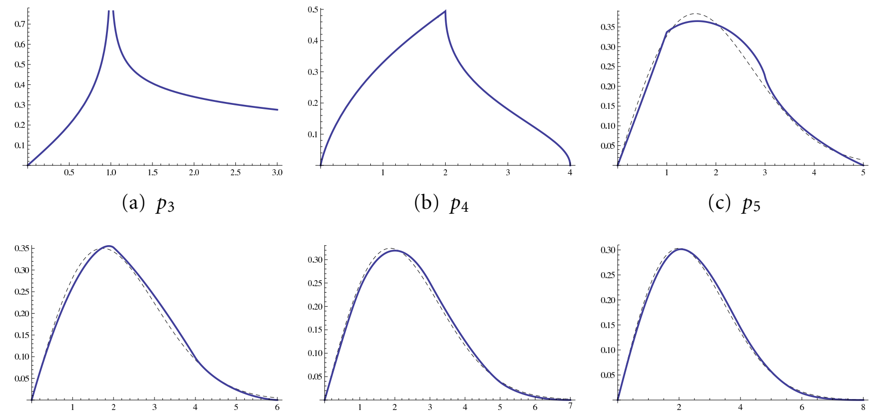

(a) p_3 (b) p_4 (c) p_5

(d) p_6 (e) p_7 (f) p_8

Figure 1: Densities p_n with the limiting behaviour superimposed for $n \geqslant 5$.

see, *e.g.*, [Pea06]. One of the main results of this paper is a closed form evaluation of p_4 as a hypergeometric function given in Theorem 4.9. In (3.4) we also provide a single hypergeometric closed form for p_3, which, in contrast to (1.2), is real and valid on all of $[0,3]$. For convenience, we list these two closed forms here:

$$p_3(x) = \frac{2\sqrt{3}}{\pi}\,\frac{x}{(3+x^2)}\,{}_2F_1\left(\left.\begin{matrix}\frac{1}{3},\frac{2}{3}\\ 1\end{matrix}\,\right|\,\frac{x^2(9-x^2)^2}{(3+x^2)^3}\right),$$

$$p_4(x) = \frac{2}{\pi^2}\,\frac{\sqrt{16-x^2}}{x}\,\mathrm{Re}\,{}_3F_2\left(\left.\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{5}{6},\frac{7}{6}\end{matrix}\,\right|\,\frac{(16-x^2)^3}{108x^4}\right).$$

We note that while *Maple* handled these well to high precision, *Mathematica* struggled, especially with the analytic continuation of the ${}_3F_2$ when the argument is greater than 1.

A striking feature of the 3- and 4-step random walk densities is their modularity. It is this circumstance which not only allows us to express them via hypergeometric series, but also makes them a remarkable object of mathematical study.

This paper is structured as follows: In Section 2 we give general results for the densities p_n and prove for instance that they satisfy certain linear differential equations. In Sections 3, 4, and 5 we provide special results for p_3, p_4, and p_5, respectively. Particular interest is taken in the behaviour near the points where the densities fail to be smooth. In Section 6 we study the derivatives of the moment function and make a connection to multidimensional Mahler measures. Finally, in Section 7 we provide some related new evaluations of moments and so resolve a central case of an earlier conjecture on convolutions of moments in [BSW11].

The amazing story of the appearance of Theorem 2.7 is worth mentioning here. The theorem was a conjecture in an earlier version of this manuscript, and one of the present authors communicated it to D. Zagier. That author was surprised to learn that Zagier had already been asked for a proof of exactly the same identities a little earlier by P. Djakov and B. Mityagin.

Those authors had in fact proved the theorem already in 2004 (see [DM04, Theorem 4.1] and [DM07, Theorem 8]) during their study of the asymptotics of the spectral gaps of a Schrödinger operator with a two-term potential. Their proof was indirect, so that we should never have come across the identities without the accident of asking the same person the same question! Djakov and Mityagin asked Zagier about the possibility of a direct proof of their identities (the subject of Theorem 2.7), and he gave a very neat and purely combinatorial answer. It is that proof which is herein presented in the Appendix.

We close this introduction with a historical remark illustrating the fascination arising from these densities and their curious geometric features. H. Fettis devotes the entire paper [Fet63] to proving that p_5 is not linear on the initial interval $[0, 1]$ as ruminated upon by Pearson [Pea06]. This will be explained in Section 5.

2 The Densities p_n

It is a classical result of Kluyver [Klu05] that p_n has the following Bessel integral representation:

$$p_n(x) = \int_0^\infty xt\, J_0(xt)\, J_0^n(t)\,\mathrm{d}t. \tag{2.1}$$

Here J_ν is the *Bessel function of the first kind* of order ν.

Remark 2.1 Equation (2.1) naturally generalizes to the case of nonuniform step lengths. In particular, for $n = 2$ and step lengths a and b we record (see [Wat44, p. 411] or [Hug95, 2.3.2]; the result is attributed to Sonine) that the corresponding density is

$$\begin{aligned} p_2(x; a, b) &= \int_0^\infty xt\, J_0(xt)\, J_0(at)\, J_0(bt)\,\mathrm{d}t \\ &= \frac{2x}{\pi\sqrt{((a+b)^2 - x^2)(x^2 - (a-b)^2)}} \end{aligned} \tag{2.2}$$

for $|a - b| \leqslant x \leqslant a + b$ and $p_2(x; a, b) = 0$ otherwise. Observe how (2.2) specializes to (1.1) in the case $a = b = 1$.

In the case $n = 3$ the density $p_3(x; a, b, c)$ has been evaluated by Nicholson [Wat44, p. 414] in terms of elliptic integrals directly generalizing (1.2). The corresponding extensions for four and more variables appear much less accessible.

It is visually clear from the graphs in Figure 1 that p_n is getting smoother for increasing n. This can be made precise from (2.1) using the asymptotic formula for J_0 for large arguments and dominated convergence:

Theorem 2.2 *For each integer $n \geqslant 0$, the density p_{n+4} is $\lfloor n/2 \rfloor$ times continuously differentiable.*

On the other hand, we note from Figure 1 that the only points preventing p_n from being smooth appear to be integers. This will be made precise in Theorem 2.4.

To this end, we recall a few things about the s-th moments $W_n(s)$ of the density p_n, which are given by

$$W_n(s) = \int_0^\infty x^s p_n(x)\,\mathrm{d}x = \int_{[0,1]^n} \left|\sum_{k=1}^n e^{2\pi x_k i}\right|^s \mathrm{d}x. \tag{2.3}$$

Starting with the right-hand side, these moments were investigated in [BNSW11, BSW11]. There it was shown that $W_n(s)$ admits an *analytic continuation* to all of the complex plane with poles of at most order two at certain negative integers. In particular, $W_3(s)$ has simple poles at $s = -2, -4, -6, \ldots$, and $W_4(s)$ has double poles at these integers [BNSW11, Thm. 6, Ex. 2 & 3].

Moreover, from the combinatorial evaluation

$$W_n(2k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2 \tag{2.4}$$

for integers $k \geqslant 0$, it followed that $W_n(s)$ satisfies a functional equation, as in [BNSW11, Ex. 1], coming from the inevitable recursion that exists for the right-hand side of (2.4). For instance, it satisfies

$$(s+4)^2 W_3(s+4) - 2(5s^2+30s+46)W_3(s+2) + 9(s+2)^2 W_3(s) = 0,$$

and

$$(s+4)^3 W_4(s+4) - 4(s+3)(5s^2+30s+48)W_4(s+2) + 64(s+2)^3 W_4(s) = 0. \tag{2.5}$$

The first part of equation (2.3) can be rephrased, saying that $W_n(s-1)$ is the *Mellin transform* of p_n ([ML86]). We denote this by $W_n(s-1) = \mathcal{M}\left[p_n; s\right]$. Conversely, the density p_n is the *inverse Mellin transform* of $W_n(s-1)$. We intend to exploit this relation as detailed for $n = 4$ in the following example.

Example 2.3 (Mellin transforms) For $n = 4$, the moments $W_4(s)$ satisfy the functional equation (2.5). Recall the following rules for the Mellin transform: if $F(s) = \mathcal{M}\left[f; s\right]$, then in the appropriate strips of convergence

- $\mathcal{M}\left[x^\mu f(x); s\right] = F(s+\mu)$,
- $\mathcal{M}\left[D_x f(x); s\right] = -(s-1)F(s-1)$.

Here, and below, D_x denotes differentiation with respect to x, and, for the second rule to be true, we have to assume, for instance, that f is continuously differentiable.

Thus, purely formally, we can translate the functional equation (2.5) of W_4 into the differential equation $A_4 \cdot p_4(x) = 0$, where A_4 is the operator

$$A_4 = x^4(\theta+1)^3 - 4x^2\theta(5\theta^2+3) + 64(\theta-1)^3 \tag{2.6}$$

$$= (x-4)(x-2)x^3(x+2)(x+4)D_x^3 + 6x^4(x^2-10)D_x^2 + x(7x^4-32x^2+64)D_x + (x^2-8)(x^2+8). \tag{2.7}$$

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Here $\theta = xD_x$. However, it should be noted that p_4 is not continuously differentiable. Moreover, $p_4(x)$ is approximated by a constant multiple of $\sqrt{4-x}$ as $x \to 4^-$ (see Theorem 4.1) so that the second derivative of p_4 is not even locally integrable. In particular, it does not have a Mellin transform in the classical sense.

Theorem 2.4 *Let an integer $n \geqslant 1$ be given.*

- *The density p_n satisfies a differential equation of order $n-1$.*
- *If n is even (respectively odd), then p_n is real analytic except at 0 and the even (respectively odd) integers $m \leq n$.*

Proof As illustrated for p_4 in Example 2.3, we use the Mellin transform method formally to translate the functional equation of W_n into a differential equation $A_n \cdot y(x) = 0$. Since p_n is locally integrable and compactly supported, it has a Mellin transform in the distributional sense as detailed for instance in [ML86]. It follows rigorously that p_n solves $A_n \cdot y(x) = 0$ in a distributional sense. In other words, p_n is a weak solution of this differential equation. The degree of this equation is $n-1$, because the functional equation satisfied by W_n has coefficients of degree $n-1$ as shown in [BNSW11, Thm. 1].

The leading coefficient of the differential equation (in terms of D_x as in (2.7)) turns out to be

$$x^{n-1} \prod_{2|(m-n)} (x^2 - m^2), \tag{2.8}$$

where the product is over the even or odd integers $1 \leq m \leq n$ depending on whether n is even or odd. This is discussed in Section 2.1.

Thus the leading coefficient of the differential equation is nonzero on $[0, n]$ except for 0 and the even or odd integers already mentioned. On each interval not containing these points it follows, as described for instance in [Hör90, Cor. 3.1.6], that p_n is in fact a classical solution of the differential equation. Moreover the analyticity of the coefficients, which are polynomials in our case, implies that p_n is piecewise real analytic as claimed. ∎

Remark 2.5 It is one of the basic properties of the Mellin transform, see for instance [FS09, Appendix B.7], that the asymptotic behaviour of a function at zero is determined by the poles of its Mellin transform, which lie to the left of the fundamental strip. It is shown in [BNSW11] that the poles of $W_n(s)$ occur at specific negative integers and are at most of second order. This translates into the fact that p_n has an expansion at 0 as a power series with additional logarithmic terms in the presence of double poles. This is made explicit in the case of p_4 in Example 4.3.

2.1 An Explicit Recursion

We close this section by providing details for the claim made in (2.8). Recall that the even moments $f_n(k) := W_n(2k)$ satisfy a recurrence of order $\lambda := \lceil n/2 \rceil$ with polynomial coefficients of degree $n-1$ (see [BNSW11]). An entirely explicit formula for this recurrence is given in [Ver04].

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Theorem 2.6

$$\sum_{j\geqslant 0}\Big[k^{n+1}\sum_{\alpha_1,\dots,\alpha_j}\prod_{i=1}^{j}(-\alpha_i)(n+1-\alpha_i)\Big(\frac{k-i}{k-i+1}\Big)^{\alpha_i-1}\Big]f_n(k-j)=0 \tag{2.9}$$

where the sum is over all sequences $\alpha_1,\dots,\alpha_j$ *such that* $0\leqslant\alpha_i\leqslant n$ *and* $\alpha_{i+1}\leqslant\alpha_i-2$.

Observe that (2.8) is easily checked for each fixed n by applying Theorem 2.6. We explicitly checked the cases $n\leqslant 1000$ (using a recursive formulation of Theorem 2.6 from [Ver04]) while only using this statement for $n\leqslant 5$ in this paper. The fact that (2.8) is true in general is recorded and made more explicit in Theorem 2.7 below.

For fixed n, write the recurrence for $f_n(k)$ in the form $\sum_{j=0}^{n-1}k^jq_j(K)$ where q_j are polynomials and K is the shift $k\to k+1$. Then q_{n-1} is the characteristic polynomial of this recurrence, and, by the rules outlined in Example 2.3, we find that the differential equation satisfied by $p_n(x)$ is of the form $q_{n-1}(x^2)\theta^{n-1}+\cdots$, where $\theta=xD_x$ and the dots indicate terms of lower order in θ.

We claim that the characteristic polynomial of the recurrence (2.9) satisfied by $f_n(k)$ is $\prod_{2|(m-n)}(x-m^2)$ where the product is over the integers $1\leq m\leq n$ such that $m\equiv n$ modulo 2. This implies (2.8). By Theorem 2.6 the characteristic polynomial is

$$\sum_{j=0}^{\lambda}\Big[\sum_{\alpha_1,\dots,\alpha_j}\prod_{i=1}^{j}(-\alpha_i)(n+1-\alpha_i)\Big]x^{\lambda-j}$$

where $\lambda=\lceil n/2\rceil$ and the sum is again over all sequences $\alpha_1,\dots,\alpha_j$ such that $0\leqslant\alpha_i\leqslant n$ and $\alpha_{i+1}\leqslant\alpha_i-2$. The claimed evaluation is thus equivalent to the following identity, first proven by P. Djakov and B. Mityagin [DM04, DM07]. Zagier's more direct and purely combinatorial proof is given in the Appendix.

Theorem 2.7 *For all integers* $n,j\geqslant 1$,

$$\sum_{\substack{0\leqslant m_1,\dots,m_j<n/2\\ m_i<m_{i+1}}}\prod_{i=1}^{j}(n-2m_i)^2=\sum_{\substack{1\leqslant\alpha_1,\dots,\alpha_j\leqslant n\\ \alpha_i\leqslant\alpha_{i+1}-2}}\prod_{i=1}^{j}\alpha_i(n+1-\alpha_i).$$

3 The Density p_3

The elliptic integral evaluation (1.2) of p_3 is very suitable to extract information about the features of p_3 exposed in Figure 1(a). It follows, for instance, that p_3 has a singularity at 1. Moreover, using the known asymptotics for $K(x)$, we may deduce that the singularity is of the form

$$p_3(x)=\frac{3}{2\pi^2}\log\Big(\frac{4}{|x-1|}\Big)+O(1) \tag{3.1}$$

as $x\to 1$.

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We also recall from [BSW11, Ex. 5] that p_3 has the expansion, valid for $0 \leqslant x \leqslant 1$,

$$p_3(x) = \frac{2x}{\pi\sqrt{3}} \sum_{k=0}^{\infty} W_3(2k)\left(\frac{x}{3}\right)^{2k} \tag{3.2}$$

where

$$W_3(2k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{2j}{j}$$

is the sum of squares of trinomials. Moreover, we have from [BSW11, Eq. 29] the functional relation

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\, p_3\left(\frac{3-x}{1+x}\right) \tag{3.3}$$

so that (3.2) determines p_3 completely and also makes apparent the behaviour at 3.

We close this section with two additional alternative expressions for p_3.

Example 3.1 (Hypergeometric form for p_3) Using the techniques in [CZ10] we can deduce from (3.2) that

$$p_3(x) = \frac{2\sqrt{3}x}{\pi(3+x^2)}\, {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right), \tag{3.4}$$

which is found in a similar but simpler way than the hypergeometric form of p_4 given in Theorem 4.9. Once obtained, this identity is easily proved using the differential equation from Theorem 2.4 satisfied by p_3. From (3.4) we see, for example, that $p_3(\sqrt{3})^2 = \frac{3}{2\pi^2} W_3(-1)$.

Example 3.2 (Iterative form for p_3) The expression (3.4) can be interpreted in terms of the cubic AGM, AG_3 (see [BB91]) as follows. Recall that $\mathrm{AG}_3(a,b)$ is the limit of iterating

$$a_{n+1} = \frac{a_n + 2b_n}{3}, \quad b_{n+1} = \sqrt[3]{b_n\left(\frac{a_n^2 + a_n b_n + b_n^2}{3}\right)},$$

beginning with $a_0 = a$ and $b_0 = b$. The iterations converge cubically, thus allowing for very efficient high-precision evaluation. On the other hand,

$$\frac{1}{\mathrm{AG}_3(1,s)} = {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; 1 - s^3\right),$$

so that as a consequence of (3.4), for $0 \leqslant x \leqslant 3$,

$$p_3(x) = \frac{2\sqrt{3}}{\pi} \frac{x}{\mathrm{AG}_3(3+x^2, 3|1-x^2|^{2/3})}.$$

Note that $p_3(3) = \frac{\sqrt{3}}{2\pi}$ is a direct consequence of the final formula.

Finally we remark that the cubic AGM also makes an appearance in the case $n = 4$. The modular properties of p_4 recorded in Remark 4.11 can be stated in terms of the theta functions

$$b(\tau) = \frac{\eta(\tau)^3}{\eta(3\tau)}, \quad c(\tau) = 3\frac{\eta(3\tau)^3}{\eta(\tau)},$$

where η is the Dedekind eta function defined in (4.14). For more information and proper definitions of the functions b, c as well as a, which is related by $a^3 = b^3 + c^3$, we refer the reader to [BBG94]. Ultimately we are hopeful that, the search for an analogue of (3.3) for p_4 may lead to an algebraic relation between the algebraically related arguments of p_4.

4 The Density p_4

The densities p_n are recursively related. As in [Hug95], setting $\phi_n(x) = p_n(x)/(2\pi x)$, we have that for integers $n \geqslant 2$,

$$\phi_n(x) = \frac{1}{2\pi}\int_0^{2\pi} \phi_{n-1}\left(\sqrt{x^2 - 2x\cos\alpha + 1}\right) \mathrm{d}\alpha.$$

We use this recursive relation to get some quantitative information about the behaviour of p_4 at $x = 4$.

Theorem 4.1 *As $x \to 4^-$,*

$$p_4(x) = \frac{\sqrt{2}}{\pi^2}\sqrt{4-x} - \frac{3\sqrt{2}}{16\pi^2}(4-x)^{3/2} + \frac{23\sqrt{2}}{512\pi^2}(4-x)^{5/2} + O\left((4-x)^{7/2}\right).$$

Proof Set $y = \sqrt{x^2 - 2x\cos\alpha + 1}$. For $2 < x < 4$,

$$\phi_4(x) = \frac{1}{\pi}\int_0^{\pi} \phi_3(y)\,\mathrm{d}\alpha = \frac{1}{\pi}\int_0^{\arccos(\frac{x^2-8}{2x})} \phi_3(y)\,\mathrm{d}\alpha,$$

since ϕ_3 is only supported on $[0, 3]$. Note that $\phi_3(y)$ is continuous and bounded in the domain of integration. By the Leibniz integral rule, we can thus differentiate under the integral sign to obtain

$$\phi_4'(x) = -\frac{1}{\pi}\frac{(x^2+8)\,\phi_3(3)}{x\sqrt{(16-x^2)(x^2-4)}} + \frac{1}{\pi}\int_0^{\arccos(\frac{x^2-8}{2x})} (x - \cos(\alpha))\,\frac{\phi_3'(y)}{y}\,\mathrm{d}\alpha. \tag{4.1}$$

This shows that ϕ_4', and hence p_4', have a singularity at $x = 4$. More specifically,

$$\phi_4'(x) = -\frac{1}{8\sqrt{2}\pi^3\sqrt{4-x}} + O(1) \quad \text{as } x \to 4^-.$$

Here, we used that $\phi_3(3) = \frac{\sqrt{3}}{12\pi^2}$. It follows that

$$p_4'(x) = -\frac{1}{\sqrt{2}\pi^2\sqrt{4-x}} + O(1),$$

which, upon integration, is the claim to first order. Differentiating (4.1) twice more proves the claim. ■

Remark 4.2 The situation for the singularity at $x = 2^+$ is more complicated, since in (4.1) both the integral (via the logarithmic singularity of ϕ_3 at 1; see (3.1)) and the boundary term contribute. Numerically, we find, as $x \to 2^+$,

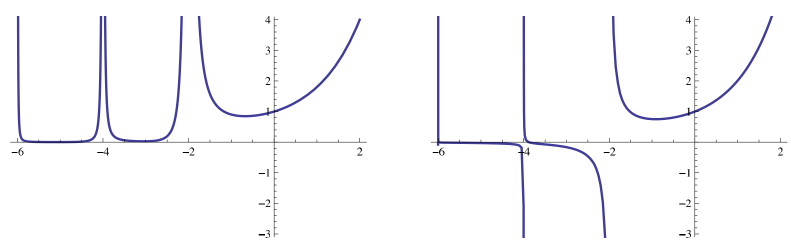
$$p_4'(x) = -\frac{2}{\pi^2\sqrt{x-2}} + O(1).$$

On the other hand, the derivative of p_4 at 2 from the left is given by

$$p_4'(2^-) = \frac{\sqrt{3}}{\pi}\, {}_3F_2\left(\left.\begin{matrix} -\frac{1}{2}, \frac{1}{3}, \frac{2}{3} \\ 1, 1 \end{matrix}\,\right|\, 1\right) - \frac{2}{3}\, p_4(2).$$

These observations can be proved in hindsight using Theorem 4.7.

We now turn to the behaviour of p_4 at zero, which we derive from the pole structure of W_4 as described in Remark 2.5.



(a) W_4 (b) W_5

Figure 2: W_4 and W_5 analytically continued to the real line.

Example 4.3 From [BSW11], we know that W_4 has a pole of order 2 at -2 as illustrated in Figure 2(a). More specifically, results in Section 6 give

$$W_4(s) = \frac{3}{2\pi^2}\frac{1}{(s+2)^2} + \frac{9}{2\pi^2}\log(2)\frac{1}{s+2} + O(1)$$

as $s \to -2$. It therefore follows that

$$p_4(x) = -\frac{3}{2\pi^2}x\log(x) + \frac{9}{2\pi^2}\log(2)x + O(x^3)$$

as $x \to 0$.

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More generally, W_4 has poles of order 2 at $-2k$ for k a positive integer. Define $s_{4,k}$ and $r_{4,k}$ by

$$W_4(s) = \frac{s_{4,k-1}}{(s+2k)^2} + \frac{r_{4,k-1}}{s+2k} + O(1) \tag{4.2}$$

as $s \to -2k$. We thus obtain that, as $x \to 0^+$,

$$p_4(x) = \sum_{k=0}^{K-1} x^{2k+1}\bigl(r_{4,k} - s_{4,k}\log(x)\bigr) + O(x^{2K+1}).$$

In fact, knowing that p_4 solves the linear Fuchsian differential equation (2.6) with a regular singularity at 0, we may conclude the following.

Theorem 4.4 *For small values $x > 0$,*

$$p_4(x) = \sum_{k=0}^{\infty}\bigl(r_{4,k} - s_{4,k}\log(x)\bigr)\, x^{2k+1}. \tag{4.3}$$

Note that

$$s_{4,k} = \frac{3}{2\pi^2}\frac{W_4(2k)}{8^{2k}}$$

as the two sequences satisfy the same recurrence and initial conditions. The numbers $W_4(2k)$ are also known as the Domb numbers ([BBBG08]), and their generating function in hypergeometric form is given in [Rog09] and has been further studied in [CZ10]. We thus have

$$\sum_{k=0}^{\infty} s_{4,k}\, x^{2k+1} = \frac{6x}{\pi^2(4-x^2)}\, {}_3F_2\left(\left.\begin{matrix}\frac13, \frac12, \frac23\\ 1, 1\end{matrix}\,\right|\, \frac{108x^2}{(x^2-4)^3}\right), \tag{4.4}$$

which is readily verified to be an analytic solution to the differential equation satisfied by p_4.

Remark 4.5 For future use, we note that (4.4) can also be written as

$$\sum_{k=0}^{\infty} s_{4,k}\, x^{2k+1} = \frac{24x}{\pi^2(16-x^2)}\, {}_3F_2\left(\left.\begin{matrix}\frac13, \frac12, \frac23\\ 1, 1\end{matrix}\,\right|\, \frac{108x^4}{(16-x^2)^3}\right), \tag{4.5}$$

which follows from the transformation

$$(1-4x)\,{}_3F_2\left(\left.\begin{matrix}\frac13, \frac12, \frac23\\ 1, 1\end{matrix}\,\right|\, -\frac{108x}{(1-16x)^3}\right) = (1-16x)\,{}_3F_2\left(\left.\begin{matrix}\frac13, \frac12, \frac23\\ 1, 1\end{matrix}\,\right|\, \frac{108x^2}{(1-4x)^3}\right)$$

given in [CZ10, (3.1)].

On the other hand, as a consequence of (4.2) and the functional equation (2.5) satisfied by W_4, the residues $r_{4,k}$ can be obtained from the recurrence relation

$$\begin{aligned}128k^3 r_{4,k} &= 4(2k-1)(5k^2-5k+2)r_{4,k-1} - 2(k-1)^3 r_{4,k-2} \\ &\quad + 3\big(64k^2 s_{4,k} - (20k^2-20k+6)s_{4,k-1} + (k-1)^2 s_{4,k-2}\big)\end{aligned}$$

with $r_{4,-1} = 0$ and $r_{4,0} = \frac{9}{2\pi^2}\log(2)$.

Remark 4.6 In fact, before realizing the connection between the Mellin transform and the behaviour of p_4 at 0, we empirically found that p_4 on $(0,2)$ should be of the form $r(x) - s(x)\log(x)$, where a and r are odd and analytic. We then numerically determined the coefficients and observed the relation with the residues of W_4 as given in Theorem 4.4.

The differential equation for p_4 has a regular singularity at 0. A basis of solutions at 0 can therefore be obtained via the Frobenius method; see for instance [Inc26]. Since the indicial equation has 1 as a triple root, the solution (4.4) is the unique analytic solution at 0, while the other solutions have a logarithmic or double logarithmic singularity. The solution with a logarithmic singularity at 0 is explicitly given in (4.8), and, from (4.3), it is clear that p_4 on $(0,2)$ is a linear combination of the analytic and the logarithmic solution.

Moreover, the differential equation for p_4 is a symmetric square. In other words, it can be reduced to a second order differential equation, which after a quadratic substitution, has 4 regular singularities and is thus of Heun type. In fact, a hypergeometric representation of p_4 with rational argument is possible.

Theorem 4.7 *For* $2 < x < 4$,

$$p_4(x) = \frac{2}{\pi^2}\frac{\sqrt{16-x^2}}{x}\,{}_3F_2\left(\begin{matrix}\frac12,\frac12,\frac12\\ \frac56,\frac76\end{matrix}\,\middle|\,\frac{(16-x^2)^3}{108x^4}\right). \tag{4.6}$$

Proof Denote the right-hand side of (4.6) by $q_4(x)$ and observe that the hypergeometric series converges for $2 < x < 4$. It is routine to verify that q_4 is a solution of the differential equation $A_4 \cdot y(x) = 0$ given in (2.6), which is also satisfied by p_4 as proved in Theorem 2.4. Together with the boundary conditions supplied by Theorem 4.1 it follows that $p_4 = q_4$. ■

We note that Theorem 4.7 gives $2\sqrt{16-x^2}/(\pi^2 x)$ as an approximation to $p_4(x)$ near $x = 4$, which is much more accurate than the elementary estimates established in Theorem 4.1.

Corollary 4.8 *In particular,*

$$p_4(2) = \frac{2^{7/3}\pi}{3\sqrt{3}}\,\Gamma\Big(\frac{2}{3}\Big)^{-6} = \frac{\sqrt{3}}{\pi}\,W_3(-1).$$

Quite marvelously, we have the following theorem, first discovered numerically.

Theorem 4.9 *For* $0 < x < 4$,

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16-x^2}}{x} \operatorname{Re} {}_3F_2\left(\left. \begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \right| \frac{(16-x^2)^3}{108x^4} \right). \tag{4.7}$$

Proof To obtain the analytic continuation of the ${}_3F_2$ for $0 < x < 2$ we employ the formula [Luk69, 5.3], valid for all z,

$$\begin{aligned} {}_{q+1}F_q\left(\left. \begin{matrix} a_1, \dots, a_{q+1} \\ b_1, \dots, b_q \end{matrix} \right| z \right) &= \frac{\prod_j \Gamma(b_j)}{\prod_j \Gamma(a_j)} \sum_{k=1}^{q+1} \frac{\Gamma(a_k) \prod_{j \neq k} \Gamma(a_j - a_k)}{\prod_j \Gamma(b_j - a_k)} (-z)^{-a_k} \\ &\quad \times {}_{q+1}F_q\left(\left. \begin{matrix} a_k, \{a_k - b_j + 1\}_j \\ \{a_k - a_j + 1\}_{j \neq k} \end{matrix} \right| \frac{1}{z} \right), \end{aligned}$$

which requires that the a_j not differ by integers. Therefore we apply it to

$${}_3F_2\left(\left. \begin{matrix} \frac{1}{2}+\varepsilon, \frac{1}{2}, \frac{1}{2}-\varepsilon \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \right| z \right).$$

and take the limit as $\varepsilon \to 0$. This ultimately produces, for $z > 1$,

$$\begin{aligned} \operatorname{Re} {}_3F_2\left(\left. \begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \right| z \right) &= \frac{\log(108z)}{2\sqrt{3z}} {}_3F_2\left(\left. \begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \right| \frac{1}{z} \right) \\ &\quad + \frac{1}{2\sqrt{3z}} \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{1}{2})_n (\frac{2}{3})_n}{n!^3} \left(\frac{1}{z}\right)^n (5H_n - 2H_{2n} - 3H_{3n}). \end{aligned} \tag{4.8}$$

Here $H_n = \sum_{k=1}^n 1/k$ is the n-th harmonic number. Now, insert the appropriate argument for z and the factors, so the left-hand side corresponds to the claimed closed form. Observing that

$$\left(\tfrac{1}{3}\right)_n \left(\tfrac{1}{2}\right)_n \left(\tfrac{2}{3}\right)_n = \frac{(2n)!(3n)!}{108^n (n!)^2},$$

we thus find that the right-hand side of (4.7) is given by $-\log(x) S_4(x)$ plus

$$\frac{6}{\pi^2} \sum_{n=0}^{\infty} \frac{(2n)!(3n)!}{(n!)^5} \frac{x^{4n+1}}{(16-x^2)^{3n}} \left(5H_n - 2H_{2n} - 3H_{3n} + 3\log(16-x^2)\right),$$

where S_4 is the solution (analytic at 0) to the differential equation for p_4 given in (4.5). This combination can now be verified to be a formal and hence actual solution of the differential equation for p_4. Together with the boundary conditions supplied by Theorem 4.4, this proves the claim. ∎

Remark 4.10 Let us indicate how the hypergeometric expression for p_4 given in Theorem 4.7 was discovered. Consider the generating series

$$y_0(z) = \sum_{k=0}^{\infty} W_4(2k) z^k \tag{4.9}$$

of the Domb numbers, which is just a rescaled version of (4.4). Corresponding to (4.5), the hypergeometric form for this series given in [Rog09] is

$$y_0(z) = \frac{1}{1-4z}\,{}_3F_2\left(\begin{matrix}\frac{1}{3},\frac{1}{2},\frac{2}{3}\\ 1,1\end{matrix}\,\middle|\,\frac{108z^2}{(1-4z)^3}\right), \tag{4.10}$$

which converges for $|z| < 1/16$. It follows that y_0 satisfies the differential equation $B_4 \cdot y_0(z) = 0$, where

$$B_4 = 64z^2(\theta+1)^3 - 2z(2\theta+1)(5\theta^2+5\theta+2) + \theta^3$$

and $\theta = z\frac{\mathrm{d}}{\mathrm{d}z}$. Up to a change of variables this is (2.6); y_0 is the unique solution that is analytic at zero and takes the value 1 at zero. The other solutions that are not a multiple of y_0 have a single or double logarithmic singularity. Let y_1 be the solution characterized by

$$y_1(z) - y_0(z)\log(z) \in z\mathbb{Q}[[z]]. \tag{4.11}$$

Note that it follows from (4.11) as well as Theorem 4.4 together with the initial values $s_{4,0} = \frac{3}{2\pi^2}$ and $r_{4,0} = s_{4,0}\log(8)$ that p_4, for small positive argument, is given by

$$p_4(x) = -\frac{3x}{4\pi^2}\, y_1\left(\frac{x^2}{64}\right). \tag{4.12}$$

If $x \in (2,4)$ and $z = x^2/64$, then the argument $t = \frac{108z^2}{(1-4z)^3}$ of the hypergeometric function in (4.10) takes the values $(1,\infty)$. We therefore consider the solutions of the corresponding hypergeometric equation at infinity. A standard basis for these is

$$t^{-1/3}{}_3F_2\left(\begin{matrix}\frac{1}{3},\frac{1}{3},\frac{1}{3}\\ \frac{2}{3},\frac{5}{6}\end{matrix}\,\middle|\,\frac{1}{t}\right),\quad t^{-1/2}{}_3F_2\left(\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{5}{6},\frac{7}{6}\end{matrix}\,\middle|\,\frac{1}{t}\right),\quad t^{-2/3}{}_3F_2\left(\begin{matrix}\frac{2}{3},\frac{2}{3},\frac{2}{3}\\ \frac{4}{3},\frac{7}{6}\end{matrix}\,\middle|\,\frac{1}{t}\right).$$

In fact, the second element suffices to express p_4 on the interval $(2,4)$ as shown in Theorem 4.7.

We close this section by showing that, remarkably, p_4 has modular structure.

Remark 4.11 As shown in [CZ10] the series y_0 defined in (4.9) possesses the modular parameterization

$$y_0\left(-\frac{\eta(2\tau)^6\eta(6\tau)^6}{\eta(\tau)^6\eta(3\tau)^6}\right) = \frac{\eta(\tau)^4\eta(3\tau)^4}{\eta(2\tau)^2\eta(6\tau)^2}. \tag{4.13}$$

Here η is the *Dedekind eta function* defined as

$$\eta(\tau) = q^{1/24}\prod_{n=1}^{\infty}(1-q^n) = q^{1/24}\sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n+1)/2}, \tag{4.14}$$

where $q = e^{2\pi i\tau}$. Moreover, the quotient of the logarithmic solution y_1, defined in (4.11), and y_0 are related to the modular parameter τ used in (4.13) by

$$\exp\left(\frac{y_1(z)}{y_0(z)}\right) = e^{(2\tau+1)\pi i} = -q. \tag{4.15}$$

Combining (4.13), (4.15), and (4.12) one obtains the modular representation

$$p_4\left(8i\frac{\eta(2\tau)^3\eta(6\tau)^3}{\eta(\tau)^3\eta(3\tau)^3}\right) = \frac{6(2\tau+1)}{\pi}\eta(\tau)\eta(2\tau)\eta(3\tau)\eta(6\tau), \tag{4.16}$$

which is valid when the argument of p_4 is small and positive. This is the case for $\tau = -1/2 + iy$ when $y > 0$. Remarkably, the argument attains the value 1 at the quadratic irrationality $\tau = (\sqrt{-5/3} - 1)/2$ (the 5/3-rd singular value of the next section). As a consequence, the value $p_4(1)$ has a nice evaluation, which is given in Theorem 5.1.

5 The Density p_5

As shown in [BSW11], $W_5(s)$ has simple poles at $-2, -4, \dots$, (compare Figure 2(b)). We write $r_{5,k} = \operatorname{Res}_{-2k-2} W_5$ for the residue of W_5 at $s = -2k-2$. A surprising bonus is an evaluation of $r_{5,0} = p_4(1) \approx 0.3299338011$, the residue at $s = -2$. This is because in general for $n \geqslant 4$, one has

$$\operatorname{Res}_{-2} W_{n+1} = p'_{n+1}(0) = p_n(1),$$

as follows from [BSW11, Prop. 1(b)]; here $p'_{n+1}(0)$ denotes the derivative from the right at zero.

Explicitly, using Theorem 4.9, we have,

$$r_{5,0} = p'_5(0) = \frac{2\sqrt{15}}{\pi^2}\operatorname{Re}{}_3F_2\left(\begin{matrix}\frac12, \frac12, \frac12\\ \frac56, \frac76\end{matrix}\,\middle|\,\frac{125}{4}\right).$$

In fact, based on the modularity of p_4 discussed in Remark 4.11 we have the following theorem.

Theorem 5.1

$$r_{5,0} = \frac{1}{2\pi^2}\sqrt{\frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{5\Gamma(\frac{7}{15})\Gamma(\frac{11}{15})\Gamma(\frac{13}{15})\Gamma(\frac{14}{15})}}. \tag{5.1}$$

Proof The value $\tau = (\sqrt{-5/3}-1)/2$ in (4.16) gives the value $p_4(1) = r_{5,0}$. Applying the Chowla–Selberg formula [SC67, BB98] to evaluate the eta functions yields the claimed evaluation. ∎

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Using [BZ92, Table 4, (ii)], (5.1) may be simplified to

$$(5.2)\quad r_{5,0} = \frac{\sqrt{5}}{40}\frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4} = \frac{3\sqrt{5}}{\pi^3}\frac{\left(\sqrt{5}-1\right)}{2}K_{15}^2 = \frac{\sqrt{15}}{\pi^3}K_{5/3}K_{15},$$

where K_{15} and $K_{5/3}$ are the complete elliptic integral at the 15-th and 5/3-rd singular values [BB98].

Remarkably, these evaluations appear to extend to $r_{5,1} \approx 0.006616730259$, the residue at $s = -4$. Resemblance to *the tiny nome of Bologna* [BBBG08] led us to discover — and then check to 400 places using (6.2) and (6.3) — that

$$(5.3)\quad r_{5,1} \stackrel{?}{=} \frac{13}{1800\sqrt{5}}\frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4} - \frac{1}{\sqrt{5}}\frac{\Gamma(\frac{7}{15})\Gamma(\frac{11}{15})\Gamma(\frac{13}{15})\Gamma(\frac{14}{15})}{\pi^4}.$$

Using (5.2) this evaluation can be neatly restated as

$$r_{5,1} \stackrel{?}{=} \frac{13}{225}r_{5,0} - \frac{2}{5\pi^4}\frac{1}{r_{5,0}}.$$

We summarize our knowledge as follows.

Theorem 5.2 *The density p_5 is real analytic on $(0,5)$ except at 1 and 3 and satisfies the differential equation $A_5 \cdot p_5(x) = 0$, where A_5 is the operator*

$$(5.4)\qquad A_5 = x^6(\theta+1)^4 - x^4(35\theta^4+42\theta^2+3) + x^2\left(259(\theta-1)^4+104(\theta-1)^2\right) - \left(15(\theta-3)(\theta-1)\right)^2$$

and $\theta = xD_x$. Moreover, for small $x > 0$,

$$(5.5)\qquad p_5(x) = \sum_{k=0}^{\infty} r_{5,k}\, x^{2k+1},$$

where

$$(5.6)\quad \left(15(2k+2)(2k+4)\right)^2 r_{5,k+2} = \left(259(2k+2)^4+104(2k+2)^2\right) r_{5,k+1} - \left(35(2k+1)^4+42(2k+1)^2+3\right) r_{5,k} + (2k)^4 r_{5,k-1}$$

with explicit initial values $r_{5,-1} = 0$ and $r_{5,0}$, $r_{5,1}$ given by (5.2) *and* (5.3).

Proof First, the differential equation (5.4) is computed in the same way as the one for p_4; see (2.6). Next, as detailed in [BSW11, Ex. 3] the residues satisfy the recurrence relation (5.6) with the given initial values. Finally, proceeding as for (4.3), we deduce that (5.5) holds for small $x > 0$. ∎

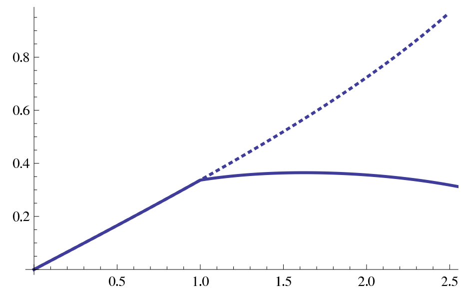

Figure 3: The series (52) (dotted) and p_5.

Numerically, the series (5.5) appears to converge for $|x| < 3$, which is in accordance with $\frac{1}{9}$ being a root of the characteristic polynomial of the recurrence (5.6); see also (2.8). The series (5.5) is depicted in Figure 3.

Since the poles of W_5 are simple, no logarithmic terms are involved in (5.5) as opposed to (4.3). In particular, by computing a few more residues from (5.6),

$$p_5(x) = 0.329934\,x + 0.00661673\,x^3 + 0.000262333\,x^5 + 0.0000141185\,x^7 + O(x^9)$$

near 0 (with each coefficient given to six digits of precision only), explaining the strikingly straight shape of $p_5(x)$ on $[0, 1]$. This phenomenon was observed by Pearson [Pea06] who stated that for $p_5(x)/x$ between $x = 0$ and $x = 1$,

> "the graphical construction, however carefully reinvestigated, did not permit of our considering the curve to be anything but a *straight* line... Even if it is not absolutely true, it exemplifies the extraordinary power of such integrals of J products [that is, (2.1)] to give extremely close approximations to such simple forms as horizontal lines."

This conjecture was investigated in detail in [Fet63] wherein the nonlinearity was first rigorously established. This work and various more recent papers highlight the difficulty of computing the underlying Bessel integrals.

Remark 5.3 Recall from Example 4.3 that the asymptotic behaviour of p_n at zero is determined by the poles of the moments $W_n(s)$. To obtain information about the behaviour of $p_n(x)$ as $x \to n^-$, we consider the "reversed" densities $\widetilde{p}_n(x) = p_n(n-x)$ and their moments $\widetilde{W}_n(s)$. For non-negative integers k,

$$\widetilde{W}_n(k) = \int_0^n x^k \widetilde{p}_n(x)\,\mathrm{d}x = \int_0^n (n-x)^k p_n(x)\,\mathrm{d}x = \sum_{j=0}^{k} \binom{k}{j} (-1)^j n^{k-j} W_n(j)$$

On the other hand, we can find a recurrence satisfied by the $\widetilde{W}_n(s)$ as follows: a differential equation for the densities $\widetilde{p}_n(x)$ is obtained from Theorem 2.4 by a change of variables. The Mellin transform method as described in Example 2.3 then provides a

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recurrence for the moments $\widetilde{W}_n(s)$. We next apply the same reasoning as in [BSW11] to obtain information about the pole structure of $\widetilde{W}_n(s)$. It should be emphasized that this involves knowledge about initial conditions in term of explicit values of initial moments $W_n(2k)$.

For instance, in the case $n = 4$, we find that the moments $\widetilde{W}_4(s)$ have simple poles at $-\frac{3}{2}, -\frac{5}{2}, -\frac{7}{2}, \dots$, which predicts an expansion of $p_4(x)$ as given in Theorem 4.1.

For $n = 5$, we learn that $\widetilde{W}_5(s)$ has simple poles at $s = -2, -3, -4, \dots$. It then follows, as for (5.5), that $p_5(x) = \sum_{k=0}^{\infty} \widetilde{r}_{5,k}\,(x-5)^{k+1}$ for $x \leqslant 5$ and close to 5. The $\widetilde{r}_{5,k}$ are the residues of $\widetilde{W}_5(s)$ at $s = -k-2$.

6 Derivative Evaluations of W_n

As illustrated by Theorem 4.4, the residues of $W_n(s)$ are very important for studying the densities p_n as they directly translate into behaviour of p_n at 0. The residues may be obtained as a linear combination of the values of $W_n(s)$ and $W_n'(s)$.

Example 6.1 (Residues of W_n) Using the functional equation for $W_3(s)$ and L'Hôpital's rule, we find that the residue at $s = -2$ can be expressed as

$$\operatorname{Res}_{-2}(W_3) = \frac{8 + 12W_3'(0) - 4W_3'(2)}{9}. \tag{6.1}$$

This is a general principle, and we likewise obtain, for instance,

$$\operatorname{Res}_{-2}(W_5) = \frac{16 + 1140W_5'(0) - 804W_5'(2) + 64W_5'(4)}{225}, \tag{6.2}$$

$$\operatorname{Res}_{-4}(W_5) = \frac{26\operatorname{Res}_{-2}(W_5) - 16 - 20W_5'(0) + 4W_5'(2)}{225}. \tag{6.3}$$

In the presence of double poles, as for W_4,

$$\lim_{s\to-2}(s+2)^2 W_4(s) = \frac{3 + 4W_4'(0) - W_4'(2)}{8} \tag{6.4}$$

and for the residue:

$$\operatorname{Res}_{-2}(W_4) = \frac{9 + 18W_4'(0) - 3W_4'(2) + 4W_4''(0) - W_4''(2)}{16}. \tag{6.5}$$

Equations (6.4) and (6.5) are used in Example 4.3, and each unknown is evaluated below.

We are therefore interested in evaluations of the derivatives of W_n for even arguments.

Example 6.2 (Derivatives of W_3 and W_4) Differentiating the double integral for $W_3(s)$ (2.3) under the integral sign, we have

$$W_3'(0) = \frac{1}{2}\int_0^1\int_0^1 \log(4\sin(\pi y)\cos(2\pi x) + 3 - 2\cos(2\pi y))\,dx\,dy.$$

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Then, using

$$\int_0^1 \log(a+b\cos(2\pi x))\,\mathrm{d}x = \log\Big(\frac{1}{2}\big(a+\sqrt{a^2-b^2}\big)\Big) \quad \text{for } a>b>0,$$

we deduce

$$W_3'(0) = \int_{1/6}^{5/6} \log\big(2\sin(\pi y)\big)\,\mathrm{d}y = \frac{1}{\pi}\,\mathrm{Cl}\Big(\frac{\pi}{3}\Big),$$

where Cl denotes the *Clausen* function. Knowing as we do that the residue at $s=-2$ is $2/(\sqrt{3}\pi)$, we can thus also obtain from (6.1) that

$$W_3'(2) = 2+\frac{3}{\pi}\,\mathrm{Cl}\Big(\frac{\pi}{3}\Big)-\frac{3\sqrt{3}}{2\pi}.$$

In like fashion,

$$\begin{aligned} W_4'(0) &= \frac{3}{8\pi^2}\int_0^\pi\int_0^\pi \log\big(3+2\,\cos x+2\,\cos y+2\,\cos(x-y)\big)\,\mathrm{d}x\,\mathrm{d}y \\ &= \frac{7}{2}\frac{\zeta(3)}{\pi^2}. \end{aligned} \tag{6.6}$$

The final equality will be shown in Example 6.6. Note that we may also write

$$W_3'(0) = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{2\pi} \log\big(3+2\cos x+2\cos y+2\cos(x-y)\big)\,\mathrm{d}x\,\mathrm{d}y.$$

The similarity between $W_3'(0)$ and $W_4'(0)$ is not coincidental, but comes from applying

$$\int_0^1 \log\big((a+\cos 2\pi x)^2+(b+\sin 2\pi x)^2\big)\,\mathrm{d}x = \begin{cases} \log(a^2+b^2) & \text{if } a^2+b^2>1, \\ 0 & \text{otherwise.} \end{cases}$$

to the triple integral of $W_4'(0)$. As this reduction breaks the symmetry, we cannot apply it to $W_5'(0)$ to get a similar integral.

In general, differentiating the Bessel integral expression

$$W_n(s) = 2^{s+1-k}\frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})}\int_0^\infty x^{2k-s-1}\Big(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\Big)^k J_0^n(x)\,\mathrm{d}x,$$

obtained by David Broadhurst and discussed in [BSW11], under the integral sign gives

$$\begin{aligned} W_n'(0) &= n\int_0^\infty \Big(\log\Big(\frac{2}{x}\Big)-\gamma\Big)\,J_0^{n-1}(x)\,J_1(x)\,\mathrm{d}x \\ &= \log(2)-\gamma-n\int_0^\infty \log(x)\,J_0^{n-1}(x)\,J_1(x)\,\mathrm{d}x, \end{aligned}$$

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where γ is the *Euler–Mascheroni* constant, and

$$W_n''(0) = n\int_0^\infty \left(\log\left(\frac{2}{x}\right) - \gamma\right)^2 J_0^{n-1}(x)\,J_1(x)\,\mathrm{d}x.$$

Likewise,

$$W_n'(-1) = (\log(2) - \gamma)W_n(-1) - \int_0^\infty \log(x)\,J_0^n(x)\,\mathrm{d}x,$$

and

$$W_n'(1) = \int_0^\infty \frac{n}{x} J_0^{n-1}(x)\,J_1(x)\big(1 - \gamma - \log(2x)\big)\,\mathrm{d}x.$$

Remark 6.3 We may therefore obtain many identities by comparing the above equations to known values. For instance,

$$3\int_0^\infty \log(x)\,J_0^2(x)\,J_1(x)\,\mathrm{d}x = \log(2) - \gamma - \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right).$$

Example 6.4 (Derivatives of W_5) In the case $n = 5$,

$$W_5'(0) = 5\int_0^\infty \left(\log\left(\frac{2}{t}\right) - \gamma\right) J_0^4(t)\,J_1(t)\,\mathrm{d}t \approx 0.54441256$$

with similar but more elaborate formulae for $W_5'(2)$ and $W_5'(4)$. Observe that in general we also have

$$W_n'(0) = \log(2) - \gamma - \int_0^1 \big(J_0^n(x) - 1\big)\frac{\mathrm{d}x}{x} - \int_1^\infty J_0^n(x)\frac{\mathrm{d}x}{x},$$

which is useful numerically.

In fact, the hypergeometric representation of W_3 and W_4 first obtained in [Cra09] and recalled below also makes derivation of the derivatives of W_3 and W_4 possible.

Corollary 6.5 (Hypergeometric forms) *For s not an odd integer, we have*

$$(6.7)\quad W_3(s) = \frac{1}{2^{2s+1}}\tan\left(\frac{\pi s}{2}\right)\binom{s}{\frac{s-1}{2}}^2 {}_3F_2\left(\left.\begin{matrix}\frac12,\frac12,\frac12\\ \frac{s+3}{2},\frac{s+3}{2}\end{matrix}\,\right|\,\frac14\right) + \binom{s}{\frac{s}{2}}\,{}_3F_2\left(\left.\begin{matrix}-\frac{s}{2},-\frac{s}{2},-\frac{s}{2}\\ 1,-\frac{s-1}{2}\end{matrix}\,\right|\,\frac14\right),$$

and, if we also have $\mathrm{Re}\,s > -2$, *we have*

$$(6.8)\quad W_4(s) = \frac{1}{2^{2s}}\tan\left(\frac{\pi s}{2}\right)\binom{s}{\frac{s-1}{2}}^3 {}_4F_3\left(\left.\begin{matrix}\frac12,\frac12,\frac12,\frac{s}{2}+1\\ \frac{s+3}{2},\frac{s+3}{2},\frac{s+3}{2}\end{matrix}\,\right|\,1\right) + \binom{s}{\frac{s}{2}}\,{}_4F_3\left(\left.\begin{matrix}\frac12,-\frac{s}{2},-\frac{s}{2},-\frac{s}{2}\\ 1,1,-\frac{s-1}{2}\end{matrix}\,\right|\,1\right).$$

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Example 6.6 (Evaluation of $W_3'(0)$ and $W_4'(0)$) If we write (6.7) or (6.8) as $W_n(s) = f_1(s)F_1(s) + f_2(s)F_2(s)$, where F_1, F_2 are the corresponding hypergeometric functions, then it can be readily verified that $f_1(0) = f_2'(0) = F_2'(0) = 0$. Thus, differentiating (6.7) by appealing to the product rule we get

$$W_3'(0) = \frac{1}{\pi}\,{}_3F_2\left(\begin{matrix}\frac12, \frac12, \frac12\\ \frac32, \frac32\end{matrix}\,\middle|\,\frac14\right) = \frac{1}{\pi}\operatorname{Cl}\left(\frac{\pi}{3}\right).$$

The last equality follows from setting $\theta = \pi/6$ in the identity

$$2\sin(\theta)\,{}_3F_2\left(\begin{matrix}\frac12, \frac12, \frac12\\ \frac32, \frac32\end{matrix}\,\middle|\,\sin^2\theta\right) = \operatorname{Cl}(2\,\theta) + 2\,\theta\log(2\sin\theta).$$

Likewise, differentiating (6.8) gives

$$W_4'(0) = \frac{4}{\pi^2}\,{}_4F_3\left(\begin{matrix}\frac12, \frac12, \frac12, 1\\ \frac32, \frac32, \frac32\end{matrix}\,\middle|\,1\right) = \frac{7\zeta(3)}{2\pi^2},$$

thus verifying (6.6). In this case the hypergeometric evaluation

$${}_4F_3\left(\begin{matrix}\frac12, \frac12, \frac12, 1\\ \frac32, \frac32, \frac32\end{matrix}\,\middle|\,1\right) = \sum_{n=0}^{\infty}\frac{1}{(2n+1)^3} = \frac78\zeta(3),$$

is elementary.

Differentiating (6.7) at $s = 2$ leads to the evaluation

$${}_3F_2\left(\begin{matrix}\frac12, \frac12, \frac12\\ \frac52, \frac52\end{matrix}\,\middle|\,\frac14\right) = \frac{27}{4}\left(\operatorname{Cl}\left(\frac{\pi}{3}\right) - \frac{\sqrt{3}}{2}\right),$$

while from (6.8) at $s = 2$ we obtain

$$W_4'(2) = 3 + \frac{14\zeta(3) - 12}{\pi^2}.$$

Thus we have enough information to evaluate (6.4) (with the answer $3/(2\pi^2)$).

Note that with two such starting values, all derivatives of $W_3(s)$ or $W_4(s)$ at even s may be computed recursively.

We also note here that the same technique yields

$$\begin{aligned}(6.9)\qquad W_3''(0) &= \frac{\pi^2}{12} - \frac{2}{\pi}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}}{4^{2n}}\frac{H_{n+1/2}}{(2n+1)^2}\\ &= \frac{\pi^2}{12} + \frac{4\log(2)}{\pi}\operatorname{Cl}\left(\frac{\pi}{3}\right) - \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}}{4^{2n}}\frac{\sum_{k=0}^{n}\frac{1}{2k+1}}{(2n+1)^2},\end{aligned}$$

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and, quite remarkably,

$$(6.10)\quad W_4''(0) = \frac{\pi^2}{12} + \frac{7\zeta(3)\log(2)}{\pi^2} + \frac{4}{\pi^2}\sum_{n=0}^{\infty}\frac{H_n - 3H_{n+1/2}}{(2n+1)^3}$$
$$= \frac{24\mathrm{Li}_4\left(\frac{1}{2}\right) - 18\zeta(4) + 21\zeta(3)\log(2) - 6\zeta(2)\log^2(2) + \log^4(2)}{\pi^2},$$

where the very final evaluation is obtained from results in [BZB08, §5]. Here $\mathrm{Li}_4(1/2)$ is the *polylogarithm* of order 4, while $H_n := \gamma + \Psi(n+1)$ denotes the nth harmonic number, where Ψ is the *digamma* function. So for non-negative integers n, we have explicitly $H_n = \sum_{k=1}^n 1/k$, as before, and

$$H_{n+1/2} = 2\sum_{k=1}^{n+1}\frac{1}{2k-1} - 2\log(2).$$

An evaluation of $W_3''(0)$ in terms of polylogarithmic constants is given in [BS11]. In particular, this gives an evaluation of the sum on the right-hand side of (6.9).

Finally, the corresponding sum for $W_4''(2)$ may be split into a telescoping part and a part involving $W_4''(0)$. Therefore, it can also be written as a linear combination of the constants used in (6.10). In summary, we have all the pieces needed to evaluate (6.5), obtaining the answer $9\log(2)/(2\pi^2)$.

6.1 Relations with Mahler Measure

For a (Laurent) polynomial $f(x_1, \ldots, x_n)$, its *logarithmic Mahler measure*, see for instance [RVTV04], is defined as

$$m(f) = \int_0^1 \cdots \int_0^1 \log\left| f(e^{2\pi i t_1}, \ldots, e^{2\pi i t_n})\right| \mathrm{d}t_1 \cdots \mathrm{d}t_n.$$

Recall that the s-th moments of an n-step random walk are given by

$$W_n(s) = \int_0^1 \cdots \int_0^1 \left|\sum_{k=1}^n e^{2\pi i t_k}\right|^s \mathrm{d}t_1 \cdots \mathrm{d}t_n = \|x_1 + \cdots + x_n\|_s^s,$$

where $\|\cdot\|_p$ denotes the p-norm over the unit n-torus, and hence

$$W_n'(0) = m(x_1 + \cdots + x_n) = m(1 + x_1 + \cdots + x_{n-1}).$$

Thus the derivative evaluations in the previous sections are also Mahler measure evaluations. In particular, we rediscovered

$$W_3'(0) = \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right) = L'(\chi_{-3}, -1) = m(1 + x_1 + x_2),$$

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along with

$$W_4'(0) = \frac{7\zeta(3)}{2\pi^2} = m(1 + x_1 + x_2 + x_3),$$

which are both due to C. Smyth [RVTV04, (1.1) and (1.2)] with proofs first published in [Boy81, Appendix 1].

With this connection realized, we find the following conjectural expressions put forth by Rodriguez-Villegas, mentioned in a different form in [Fin05],

$$W_5'(0) \stackrel{?}{=} \left(\frac{15}{4\pi^2}\right)^{5/2} \int_0^\infty \left\{ \eta^3(e^{-3t})\eta^3(e^{-5t}) + \eta^3(e^{-t})\eta^3(e^{-15t}) \right\} t^3 \, \mathrm{d}t \tag{6.11}$$

and

$$W_6'(0) \stackrel{?}{=} \left(\frac{3}{\pi^2}\right)^3 \int_0^\infty \eta^2(e^{-t})\eta^2(e^{-2t})\eta^2(e^{-3t})\eta^2(e^{-6t}) \, t^4 \, \mathrm{d}t, \tag{6.12}$$

where η was defined in (4.14). We have confirmed numerically that the evaluation of $W_5'(0)$ in (6.11) holds to 600 places. Likewise, we have confirmed that (6.12) holds to 80 places. Details of these somewhat arduous confirmations are given in [BB10].

Differentiating the series expansion for $W_n(s)$ obtained in [BNSW11] term by term, we obtain

$$W_n'(0) = \log(n) - \sum_{m=1}^\infty \frac{1}{2m} \sum_{k=0}^m \binom{m}{k} \frac{(-1)^k W_n(2k)}{n^{2k}}.$$

On the other hand, from [RVTV04] we find the strikingly similar

$$W_n'(0) = \frac{1}{2}\log(n) - \frac{\gamma}{2} - \sum_{m=2}^\infty \frac{1}{2m} \sum_{k=0}^m \binom{m}{k} \frac{(-1)^k W_n(2k)}{k!\, n^k}.$$

Finally, we note that $W_n(s)$ itself is a special case of *zeta Mahler measure* as introduced in [Aka09].

7 New Results on the Moments W_n

From [BBBG08, Eq. (23)], we have for $k > 0$ even,

$$W_3(k) = \frac{3^{k+3/2}}{\pi\, 2^k\, \Gamma(k/2+1)^2} \int_0^\infty t^{k+1} K_0(t)^2 I_0(t) \mathrm{d}t, \tag{7.1}$$

where $I_0(t), K_0(t)$ denote the *modified Bessel functions* of the first and second kind, respectively.

Similarly, [BBBG08, Eq. (55)] states that for $k > 0$ even,

$$W_4(k) = \frac{4^{k+2}}{\pi^2\, \Gamma(k/2+1)^2} \int_0^\infty t^{k+1} K_0(t)^3 I_0(t) \mathrm{d}t. \tag{7.2}$$

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Equation (7.1) can be formally reduced to a closed form as a ${}_3F_2$ (for instance by *Mathematica*). At $k = \pm 1$, the closed form agrees with $W_3(\pm 1)$. As both sides of (7.1) satisfy the same recursion ([BBBG08, Eq. (8)]), we see that it in fact holds for all integers $k > -2$.

In the following we shall use Carlson's theorem ([Tit39]).

Theorem (Carlson's [Tit39]) *Let f be analytic in the right half-plane $\operatorname{Re} z \geqslant 0$ and of exponential type with the additional requirement that*

$$|f(z)| \leqslant Me^{d|z|}$$

for some $d < \pi$ on the imaginary axis $\operatorname{Re} z = 0$. If $f(k) = 0$ for $k = 0, 1, 2, \ldots$ then $f(z) = 0$ identically.

We then have the following lemma.

Lemma 7.1 *Equation* (7.1) *holds for all k with $\operatorname{Re} k > -2$.*

Proof Both sides of (7.1) are of exponential type and agree when $k = 0, 1, 2, \ldots$. The standard estimate shows that the right-hand side grows like $e^{|y|\pi/2}$ on the imaginary axis. Therefore the conditions of Carlson's theorem are satisfied and the identity holds whenever the right-hand side converges. ∎

Using the closed form given by the computer algebra system, we thus have the following theorem.

Theorem 7.2 (Single hypergeometric for $W_3(s)$) *For s not a negative integer < -1,*

$$W_3(s) = \frac{3^{s+3/2}}{2\pi} \frac{\Gamma(1+s/2)^2}{\Gamma(s+2)} \, {}_3F_2\left({\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \atop 1, \frac{s+3}{2}} \middle| \frac{1}{4} \right).$$

Turning our attention to negative integers, we have for an integer $k \geqslant 0$:

$$W_3(-2k-1) = \frac{4}{\pi^3} \left(\frac{2^k k!}{(2k)!} \right)^2 \int_0^\infty t^{2k} K_0(t)^3 \mathrm{d}t, \tag{7.3}$$

because the two sides satisfy the same recursion ([BBBG08, (8)]) and agree when $k = 0, 1$ ([BBBG08, (47) and (48)]).

Remark 7.3 Equation (7.3), however, does not hold when k is not an integer. Also, combining (7.3) and (7.1) for $W_3(-1)$, we deduce

$$\int_0^\infty K_0(t)^2 I_0(t) \, \mathrm{d}t = \frac{2}{\sqrt{3}\pi} \int_0^\infty K_0(t)^3 \, \mathrm{d}t = \frac{\pi^2}{2\sqrt{3}} \int_0^\infty J_0(t)^3 \, \mathrm{d}t.$$

From (7.3), we experimentally determine a single hypergeometric for $W_3(s)$ at negative odd integers.

Lemma 7.4 *For an integer $k \geqslant 0$,*

$$W_3(-2k-1) = \frac{\sqrt{3}\binom{2k}{k}^2}{2^{4k+1}3^{2k}}\,{}_3F_2\left(\begin{matrix}\frac12,\frac12,\frac12\\ k+1,k+1\end{matrix}\,\middle|\,\frac14\right).$$

Proof It is easy to check that both sides agree at $k = 0, 1$. Therefore we only need to show that they satisfy the same recursion. The recursion for the left-hand side implies a contiguous relation for the right-hand side, which can be verified by extracting the summand and applying Gosper's algorithm ([PWZ96]). ∎

The integral in (7.3) shows that $W_3(-2k-1)$ decays to 0 rapidly — very roughly like 9^{-k} as $k \to \infty$ — and so is never 0 when k is an integer.

To show that (7.2) holds for more general k required more work. Using Nicholson's integral representation in [Wat44],

$$I_0(t)K_0(t) = \frac{2}{\pi}\int_0^{\pi/2} K_0(2t\sin a)\,\mathrm{d}a,$$

the integral in (7.2) simplifies to

$$\frac{2}{\pi}\int_0^{\pi/2}\int_0^{\infty} t^{k+1}K_0(t)^2K_0(2t\sin a)\,\mathrm{d}t\mathrm{d}a. \tag{7.4}$$

The inner integral in (7.4) simplifies in terms of a *Meijer G-function*; *Mathematica* is able to produce

$$\frac{\sqrt{\pi}}{8\sin^{k+2}a}\,G^{3,2}_{3,3}\left(\begin{matrix}-\frac12,-\frac12,\frac12\\ 0,0,0\end{matrix}\,\middle|\,\frac{1}{\sin^2 a}\right),$$

which transforms to

$$\frac{\sqrt{\pi}}{8\sin^{k+2}a}\,G^{2,3}_{3,3}\left(\begin{matrix}1,1,1\\ \frac32,\frac32,\frac12\end{matrix}\,\middle|\,\sin^2 a\right).$$

Let $t = \sin^2 a$ in the above, so the outer integral in (7.4) transforms to

$$\frac{\sqrt{\pi}}{16}\int_0^1 t^{-\frac{k+3}{2}}(1-t)^{-\frac12}\,G^{2,3}_{3,3}\left(\begin{matrix}1,1,1\\ \frac32,\frac32,\frac12\end{matrix}\,\middle|\,t\right)\mathrm{d}t. \tag{7.5}$$

We can resolve this integral by applying the Euler-type integral

$$\int_0^1 t^{-a}(1-t)^{a-b-1}\,G^{m,n}_{p,q}\left(\begin{matrix}\mathbf{c}\\ \mathbf{d}\end{matrix}\,\middle|\,zt\right)\mathrm{d}t = \Gamma(a-b)\,G^{m,n+1}_{p+1,q+1}\left(\begin{matrix}a,\mathbf{c}\\ \mathbf{d},b\end{matrix}\,\middle|\,z\right). \tag{7.6}$$

Indeed, when $k = -1$, the application of (7.6) recovers the Meijer G representation of $W_4(-1)$ ([BSW11]); that is, (7.2) holds for $k = -1$.

When $k = 1$, the resulting Meijer G-function is

$$G^{2,4}_{4,4}\left(\begin{matrix}2,1,1,1\\ \frac32,\frac32,\frac12,\frac32\end{matrix}\,\middle|\,1\right),$$

to which we apply Nesterenko's theorem ([Nes03]), deducing a triple integral (up to a constant factor)

$$\int_0^1 \int_0^1 \int_0^1 \sqrt{\frac{x(1-x)z}{y(1-y)(1-z)(1-x(1-yz))^3}}\, \mathrm{d}x\mathrm{d}y\mathrm{d}z.$$

We can reduce the triple integral to a single integral,

$$\int_0^1 \frac{8E'(t)\big((1+t^2)K'(t)-2E'(t)\big)}{(1-t^2)^2}\, \mathrm{d}t.$$

Now applying the change of variable $t \mapsto (1-t)/(1+t)$, followed by quadratic transformations for K and E, we finally get

$$\int_0^1 \frac{4(1+t)}{t^2} E\Big(\frac{2\sqrt{t}}{1+t}\Big)\big(K(t)-E(t)\big)\, \mathrm{d}t,$$

which is, indeed, (a correct constant multiple times) the expression for $W_4(1)$, which follows from Section 3.1 in [BSW11].

We finally observe that both sides of (7.2) satisfy the same recursion ([BBBG08, Eq. (9)]), hence they agree for $k = 0, 1, 2, \dots$. Carlson's theorem applies with the same growth on the imaginary axis as in (7.1), and we have proved the following lemma.

Lemma 7.5 *Equation* (7.2) *holds for all k with* $\operatorname{Re} k > -2$.

Theorem 7.6 (Alternative Meijer G representation for $W_4(s)$) *For all s,*

$$W_4(s) = \frac{2^{2s+1}}{\pi^2\,\Gamma(\frac{1}{2}(s+2))^2}\, G^{2,4}_{4,4}\left(\begin{matrix} 1, 1, 1, \frac{s+3}{2} \\ \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2} \end{matrix} \,\middle|\, 1 \right).$$

Proof Apply (7.6) to (7.5) for general k, and the equality holds by Lemma 7.5. ∎

Note that Lemma 7.5 combined with the known formula for $W_4(-1)$ in [BSW11] gives

$$\frac{4}{\pi^3}\int_0^\infty K_0(t)^3 I_0(t)\,\mathrm{d}t = \int_0^\infty J_0(t)^4\,\mathrm{d}t.$$

Armed with the knowledge of Lemma 7.5, we may now resolve a very special but central case (corresponding to $n = 2$) of [BSW11, Conjecture 1].

Theorem 7.7 *For integer s,*

$$W_4(s) = \sum_{j=0}^{\infty} \binom{s/2}{j}^2 W_3(s-2j). \tag{7.7}$$

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Proof In [BNSW11] it is shown that both sides satisfy the same three term recurrence, and agree when s is even. Therefore, we only need to show that the identity holds for two consecutive odd values of s.

For $s = -1$, the right-hand side of (7.7) is

$$\sum_{j=0}^{\infty} \binom{-1/2}{j}^2 W_3(-1-2j) = \sum_{j=0}^{\infty} \frac{2^{2-2j}}{\pi^3 j!^2} \int_0^{\infty} t^{2j} K_0(t)^3 \, \mathrm{d}t$$

upon using (7.3), and after interchanging summation and integration (which is justified as all terms are positive), this reduces to

$$\frac{4}{\pi^3} \int_0^{\infty} K_0(t)^3 I_0(t) \, \mathrm{d}t,$$

which is the value for $W_4(-1)$ by Lemma 7.5.

We note that the recursion for $W_4(s)$ gives the pleasing reflection property

$$W_4(-2k-1)\, 2^{6k} = W_4(2k-1).$$

In particular, $W_4(-3) = \frac{1}{64} W_4(1)$. Now computing the right-hand side of (7.7) at $s = -3$ and interchanging summation and integration as before, we obtain

$$\sum_{j=0}^{\infty} \binom{-3/2}{j}^2 W_3(-3-2j) = \frac{4}{\pi^3} \int_0^{\infty} t^2 K_0(t)^3 I_0(t) \, \mathrm{d}t = \frac{1}{64} W_4(1) = W_4(-3).$$

Therefore (7.7) holds when $s = -1, -3$, and thus holds for all integer s. ■

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A Appendix. A Family of Combinatorial Identities[1]

Don Zagier

The "collateral result" of Djakov and Mityagin, [DM04, DM07], is the pair of identities

$$\sum_{\substack{-m<i_1<\cdots<i_k<m \\ i_2-i_1,\dots,i_k-i_{k-1}\geqslant 2}} \prod_{s=1}^{k}(m^2-i_s^2) = \sigma_k(1^2,3^2,\dots,(2m-1)^2)\,,$$

$$\sum_{\substack{1-m<i_1<\cdots<i_k<m \\ i_2-i_1,\dots,i_k-i_{k-1}\geqslant 2}} \prod_{s=1}^{k}(m-i_s)(m+i_s-1) = \sigma_k(2^2,4^2,\dots,(2m-2)^2)\,,$$

where m and k are integers with $m \geqslant k \geqslant 0$ and σ_k denotes the k-th elementary symmetric function. By setting $j_s = i_s + m$ in the first sum and $j_s = i_s + m - 1$ in the second, we can rewrite these formulas more uniformly as[2]

$$F_{M,k}(M) = \begin{cases} \sigma_k(1^2,3^2,\dots,(M-1)^2) & \text{if } M \text{ is even,} \\ \sigma_k(2^2,4^2,\dots,(M-1)^2) & \text{if } M \text{ is odd,} \end{cases} \tag{A.1}$$

where $F_{M,k}(X)$ is the polynomial in X (non-zero only if $M \geqslant 2k \geqslant 0$) defined by

$$F_{M,k}(X) = \sum_{\substack{0<j_1<\cdots<j_k<M \\ j_2-j_1,\dots,j_k-j_{k-1}\geqslant 2}} \prod_{s=1}^{k} j_s(X-j_s)\,. \tag{A.2}$$

The advantage of introducing the free variable X in (A.2) is that the functions $F_{M,k}(X)$ satisfy the recursion

$$F_{M+1,k+1}(X) - F_{M,k+1}(X) = M\,(X-M)\,F_{M-1,k}(X), \tag{A.3}$$

because the only paths that are counted on the left are those with $0 < j_1 < \cdots < j_k < j_{k+1} = M$.

It is also advantageous to introduce the polynomial generating function

$$\Phi_M = \Phi_M(X,u) = \sum_{0\leqslant k\leqslant M/2} (-1)^k\,F_{M,k}(X)\,u^{M-2k}\,,$$

the first examples being

$$\Phi_0 = 1, \quad \Phi_1 = u, \quad \Phi_2 = u^2-(X-1), \quad \Phi_3 = u^3-(3X-5)u,$$

$$\Phi_4 = u^4-(6X-14)u^2+(3X^2-12X+9),$$

$$\Phi_5 = u^5-(10X-30)u^3+(15X^2-80X+89),$$

$$\Phi_6 = u^6-(15X-55)u^4+(45X^2-300X+439)u^2 \\ -(15X^3-135X^2+345X-225).$$

[1]The original note is unchanged.
[2]Note that (A.1) is precisely Theorem 2.7.

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In terms of this generating function, the recursion (A.3) becomes

$$\Phi_{M+1} = u\,\Phi_M - M(X-M)\,\Phi_{M-1}, \tag{A.4}$$

and the identity (A.1) to be proved can be written succinctly as

$$\Phi_M(M,u) = \prod_{\substack{|\lambda|<M \\ \lambda\not\equiv M \pmod 2}} (u-\lambda)\,. \tag{A.5}$$

Denote by $P_M(u)$ the polynomial on the right-hand side of (A.5). Looking for other pairs (M,X), where $\Phi_M(X,u)$ has many integer roots, we find experimentally that this happens whenever $M-X$ is a non-negative integer, and studying the data more closely we conjecture two formulas:

$$\Phi_M(M-n,u) = \frac{1}{2^n}\sum_{j=0}^{n}\binom{n}{j} P_M(u-n+2j) \qquad (M,\ n\geqslant 0) \tag{A.6}$$

(a generalization of (A.5)) and

$$\Phi_{M+n}(M,u) = \Phi_M(M,u)\,\Phi_n(-M,u) \qquad (M,\ n\geqslant 0)\,. \tag{A.7}$$

Formula (A.7) is easy to prove, since it holds for $n=0$ trivially and for $n=1$ by (A.4) and since both sides satisfy the recursion $y_{n+1} = u\,y_n + n(M+n)\,y_{n-1}$ for $n=1,2,\dots$ by (A.4). On the other hand, combining (A.5), (A.6), and (A.7) leads to the conjectural formula

$$\begin{aligned}\Phi_n(-M,u) &= \frac{1}{2^n}\sum_{j=0}^{n}\binom{n}{j}\frac{P_{M+n}(u-n+2j)}{P_n(u)}\\ &= n!\sum_{j=0}^{n}(-1)^j\binom{\frac{-u-M-1}{2}}{j}\binom{\frac{u-M-1}{2}}{n-j}\end{aligned}$$

or, renaming the variables,

$$\frac{1}{M!}\,\Phi_M(x+y+1,y-x) = \sum_{j=0}^{M}(-1)^j\binom{x}{j}\binom{y}{M-j}\,.$$

To prove this, we see by (A.4) that, denoting by $G_M = G_M(x,y)$ the expression on the right, it suffices to prove the recursion

$$(M+1)G_{M+1} = (y-x)G_M + (M-x-y-1)G_{M-1}.$$

This is an easy binomial coefficient identity, but once again it is easier to work with generating functions. The sum

$$\mathcal{G}(x,y;T) := \sum_{M=0}^{\infty} G_M(x,y)\,T^m = (1-T)^x\,(1+T)^y \tag{A.8}$$

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satisfies the differential equation

$$\frac{1}{\mathcal{G}}\frac{\partial \mathcal{G}}{\partial T} = \frac{y}{1+T} - \frac{x}{1-T} \quad \text{or} \quad \frac{\partial \mathcal{G}}{\partial T} = (y-x)\,\mathcal{G} + \Big(T\frac{\partial}{\partial T} - x - y\Big)\,\mathcal{G},$$

and this is equivalent to the desired recursion.

We can now complete the proof of (A.1). Rewriting (A.8) in the form

$$\frac{1}{M!}\,\Phi_M(X,u) = \mathrm{coeff}_{T^M}\Big((1-T)^{\frac{X-u-1}{2}}\,(1+T)^{\frac{X+u-1}{2}}\Big),$$

we find that, for $1 \leqslant j \leqslant M$,

$$\frac{1}{M!}\,\Phi_M(M, M+1-2j) = \mathrm{coeff}_{T^M}\Big((1-T)^{j-1}\,(1+T)^{M-j}\Big) = 0,$$

and hence that the polynomial on the left-hand side of (A.5) is divisible by the polynomial on the right, which completes the proof since both are monic of degree M in u. ∎

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