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## On Dirichlet eigenvalues of regular polygons



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#### ABSTRACT

We prove that the first Dirichlet eigenvalue of a regular N-gon of area  $\pi$  has an asymptotic expansion of the form  $\lambda_1(1+\sum_{n\geq 3}\frac{C_n(\lambda_1)}{N^n})$  as  $N\to\infty$ , where  $\lambda_1$  is the first Dirichlet eigenvalue of the unit disk and  $C_n$  are polynomials whose coefficients belong to the space of multiple zeta values of weight n and conjecture that their coefficients lie in the space of single-valued multiple zeta values. We also explicitly compute these polynomials for all n<14.

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### 1. Introduction

Let  $\Omega$  be a bounded connected domain with piecewise smooth boundary in  $\mathbb{R}^2$  and let us denote by  $\Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$  the standard flat Laplace operator. When one considers suitable spaces of functions on  $\overline{\Omega}$  with Dirichlet boundary conditions (i.e., vanishing on  $\partial\Omega$ ) it is well known by the spectral theorem that  $\Delta$  possesses a discrete spectrum  $\{\lambda_k(\Omega)\}_{k=1}^{\infty}$  of eigenvalues

$$0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \dots$$

with corresponding finite-dimensional eigenspaces  $\text{Eig}(\lambda_k)$  of smooth eigenfunctions. In other words each eigenfunction  $\varphi \in \text{Eig}(\lambda_k)$  satisfies the following boundary value PDE:

$$\begin{cases} \Delta \varphi + \lambda_k \varphi = 0, \\ \varphi|_{\partial \Omega} = 0. \end{cases}$$

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One can consider many aspects regarding the asymptotics of Dirichlet eigenvalues and Dirichlet eigenfunctions, a large portion of which could be regarded as "classical" and being intensely studied: without aiming at being thorough, we just mention, for example, various forms of Weyl laws prescribing the asymptotics of large eigenvalues  $\lambda_k$  in terms of the underlying geometric data; concentration phenomena for eigenfunctions and level set distribution; behavior of eigenvalues with respect to domain perturbation; etc. For a very thorough and accessible overview we refer to the treatments in [8], [28].

In this note we are interested in the behavior of the eigenvalues with respect to domain perturbations in the special case of regular polygons. Let  $\mathcal{P}_N$  be a regular polygon of area  $\pi$  with  $N \geq 3$  sides. We study the behavior of  $\lambda_k(\mathcal{P}_N)$  as N goes to infinity. More precisely, we are interested in computing the coefficients  $C_{k,n}$  of the asymptotic series

$$\frac{\lambda_k(\mathcal{P}_N)}{\lambda_k(\mathbb{D})} \sim 1 + \frac{C_{k,1}}{N} + \frac{C_{k,2}}{N^2} + \frac{C_{k,3}}{N^3} + \dots,$$
 (1)

where  $\mathbb{D}$  is the unit disk.

The above problem has been considered in several previous works. As an outcome of the works [17], [11], [12] the first four coefficients  $C_{1,i}$  were computed and, to a certain surprise, expressed as integer multiples of the Riemann zeta function. Roughly speaking, the corresponding methods (Calculus of Moving Surfaces) require one to consider an explicit deformation of the polygon into a disk and study the evolution of the corresponding eigenfunction.

Later on, the next two coefficients  $C_{1,5}$ ,  $C_{1,6}$  were also computed and given in a similar form (cf. [4]). Recently, in [14] an expression for the next two coefficients  $C_{1,7}$ ,  $C_{1,8}$  was proposed as a result of high-precision numerics and certain linear regression methods.

To summarize the above results, assuming that the polygons under consideration are normalized in such a way that  $Area(\mathcal{P}_N) = \pi$ , the asymptotic expansion (with proposed seventh and eighth terms being conjectural) is the following

$$\frac{\lambda_1(\mathcal{P}_N)}{\lambda_1} = 1 + \frac{4\zeta(3)}{N^3} + \frac{(12 - 2\lambda_1)\zeta(5)}{N^5} + \frac{(8 + 4\lambda_1)\zeta^2(3)}{N^6} + \frac{(36 - 12\lambda_1 - \frac{1}{2}\lambda_1^2)\zeta(7)}{N^7} + \frac{(48 + 8\lambda_1 + 2\lambda_1^2)\zeta(3)\zeta(5)}{N^8} + O(N^{-9}).$$
(2)

Here  $\lambda_1 = \lambda_1(\mathbb{D})$  is the first Dirichlet eigenvalue of the unit disk. Recall that  $\lambda_1 = j_{0,1}^2$ , where  $j_{0,1}$  is the smallest positive zero of the Bessel function of the first kind  $J_0$ .

Formula (2) might lead one to suspect that all higher coefficients of the asymptotic expansion can be expressed as polynomials in  $\lambda_1$  with coefficients that are polynomials in odd zeta values  $\zeta(2m+1)$ ,  $m \geq 1$ . As we will show below, this is indeed the case for the first 10 coefficients of the expansion, but, assuming some widely believed algebraic independence results, the 11-th coefficient is no longer of this form.

As further motivation we note a couple of related problems. Drawing inspiration from the Faber-Krahn inequality and a conjecture of Pólya and Szegö (which states that among all n-gons with the same area, the regular n-gon has the smallest first Dirichlet eigenvalue), it was conjectured in [1] that for all  $N \geq 3$  and  $\text{Area}(\mathcal{P}_N) = \pi$ , the first Dirichlet eigenvalues are monotonically decreasing in N, i.e.,

$$\lambda_1(\mathcal{P}_N) > \lambda_1(\mathcal{P}_{N+1})$$
.

So far the monotonicity has been confirmed by numerical experiments (cf. [1]). Note, however, that since  $\zeta(3) > 0$ , equation (2) implies this inequality for all sufficiently large N. For further results along the theme of Faber-Krahn and eigenvalue optimization via regular polygons under the presence of various constraints (in- and circumradius normalization, etc.) we refer to [19], [21] and the references therein.

A further intriguing application of the above eigenvalue asymptotics can be found in [20], where the Casimir energy of a scalar field on  $\mathcal{P}_N$  (and further generalized to  $\mathcal{P}_N \times \mathbb{R}^k$ ) has been studied. For background we refer to [20] and the accompanying references.

Before describing our main results, we briefly recall the definition of multiple zeta values. Multiple zeta values (MZVs) are real numbers defined by

$$\zeta(m_1, \dots, m_r) \coloneqq \sum_{0 < n_1 < n_2 < \dots < n_r} \frac{1}{n_1^{m_1} n_2^{m_2} \dots n_r^{m_r}},$$

where  $m_1, \ldots, m_r$  are positive integers and  $m_r > 1$ . A multiple zeta value  $\zeta(m_1, \ldots, m_r)$  is said to have weight n if  $m_1 + \cdots + m_r = n$ . We denote the  $\mathbb{Q}$ -linear span of all multiple zeta values of weight n by  $\mathfrak{Z}_n$ . Our main result is the following theorem.

**Theorem 1.** There exists a sequence of polynomials  $C_n \in \mathfrak{Z}_n[\lambda]$ ,  $n \geq 1$ , where  $\mathfrak{Z}_n$  is the space of multiple zeta values of weight n, such that

$$\frac{\lambda_k(\mathcal{P}_N)}{\lambda_k} \sim 1 + \sum_{n=1}^{\infty} \frac{C_n(\lambda_k)}{N^n} \tag{3}$$

whenever  $\lambda_k$  is a radially-symmetric Dirichlet eigenvalue of the unit disk.

Here radially-symmetric eigenvalues are  $\lambda_k$ 's for which the corresponding eigenfunction is radially-symmetric. Explicitly, the theorem applies whenever  $\lambda_k = j_{0,m}^2$ , where  $j_{0,m}$  is the m-th zero of the Bessel function  $J_0(x)$ . In particular, the theorem applies in the case k = 1.

The proof of Theorem 1 is based on an asymptotic version of the "method of particular solutions" (see, e.g., [10], [18]) and it provides an explicit procedure for producing increasingly better approximations (at least when  $N \to \infty$ ) to both the eigenvalues and the eigenfunctions (as long as they correspond to the radially symmetric eigenfunctions on the unit disk). We find that not only the eigenvalues, but the eigenfunctions themselves have asymptotic expansions in powers of 1/N with interesting coefficients (these coefficients turn out to be multiple polylogarithms, see Table 2).

Our approach gives an explicit symbolic algorithm for computing the polynomials  $C_n$ . We have calculated  $C_n$  for  $n \leq 12$  using an implementation of this algorithm in the computer algebra system SAGE [22] and for  $n \leq 14$  using an optimized parallel implementation in Julia [15]. As an immediate corollary we confirm the 7-th and 8-th terms in the asymptotic expansion (1) that were conjectured in [14]. We collect the results of our calculations in Table 1. The initial expressions in terms of MZVs that we get by directly applying our algorithm are rather unwieldy and to obtain the simpler expressions given in the table we have used the MZV Datamine [3]. In the table we use the notation  $\zeta_n := \zeta(n)$  and

$$\begin{split} \zeta_{3,5,3}^{\mathrm{sv}} &\coloneqq 2\zeta(3,5,3) - 2\zeta(3)\zeta(3,5) - 10\zeta(3)^2\zeta(5)\,, \\ \zeta_{5,3,5}^{\mathrm{sv}} &\coloneqq 2\zeta(5,3,5) - 22\zeta(5)\zeta(3,5) - 120\zeta(5)^2\zeta(3) - 10\zeta(5)\zeta(8)\,, \\ \zeta_{3,7,3}^{\mathrm{sv}} &\coloneqq 2\zeta(3,7,3) - 2\zeta(3)\zeta(3,7) - 28\zeta(3)^2\zeta(7) - 24\zeta(5)\zeta(3,5) - 144\zeta(5)^2\zeta(3) - 12\zeta(5)\zeta(8) \end{split}$$

for the first few nontrivial single-valued MZVs. The space of single-valued multiple zeta values of weight n is an important subspace of  $\mathfrak{Z}_n$  that was introduced by Brown [6]. Single-valued MZVs appear, for example, in computation of string amplitudes, and as coefficients of Deligne's associator (for other examples, see the references in [6]).

Conjecture 1. The polynomial  $C_n(\lambda)$  belongs to  $\mathfrak{Z}_n^{\text{sv}}[\lambda]$  for all  $n \geq 1$ , where  $\mathfrak{Z}_n^{\text{sv}}$  denotes the space of single-valued multiple zeta values of weight n.

Table 1 Coefficients of the asymptotic expansion for  $n \leq 14$ .

```
0
1
2
                                                                                         0
3
                                                                                         4\zeta_3
4
5
                                                                                             -2\zeta_5\lambda + 12\zeta_5
                                                                                         4\zeta_2^2\lambda + 8\zeta_2^2
6
                                                                                             -\frac{1}{2}\zeta_7\lambda^2 - 12\zeta_7\lambda + 36\zeta_7
7
                                                                                         2\zeta_5\zeta_3\lambda^2 + 8\zeta_5\zeta_3\lambda + 48\zeta_5\zeta_3
                                                                                             -\frac{1}{4}\zeta_9\lambda^3 - \frac{104}{9}\zeta_9\lambda^2 + (-\frac{146}{3}\zeta_9 + \frac{80}{3}\zeta_3^3)\lambda + (\frac{340}{3}\zeta_9 + \frac{32}{3}\zeta_3^3)
                                                                                      (\zeta_7\zeta_3 + \zeta_5^2)\lambda^3 + (39\zeta_7\zeta_3 - 6\zeta_5^2)\lambda^2 + (-24\zeta_7\zeta_3 - 12\zeta_5^2)\lambda + (144\zeta_7\zeta_3 + 72\zeta_5^2)\lambda^2 + (-24\zeta_7\zeta_3 - 12\zeta_5^2)\lambda^2 + (-24\zeta_7\zeta_5 - 12\zeta_5^2)\lambda^2 + (
10
                                                                                         -\frac{5}{32}\zeta_{11}\lambda^4 + (-\frac{661}{60}\zeta_{11} + \frac{1}{5}\xi_{3,5,3}^{88})\lambda^3 + (-\frac{1623}{20}\zeta_{11} + 80\zeta_5\zeta_3^2 + \frac{54}{5}\xi_{3,5,3}^{88})\lambda^2 + (-176\zeta_{11} + 176\zeta_5\zeta_3^2)\lambda + (372\zeta_{11} + 96\zeta_5\zeta_3^2)\lambda^2 + (372\zeta_{11} + 96\zeta_5\zeta_5^2)\lambda^2 + (372\zeta_{11} + 96\zeta_5\zeta_
11
                                                                                         (\tfrac{5}{8}\zeta_9\zeta_3 + \tfrac{11}{8}\zeta_7\zeta_5)\lambda^4 + (\tfrac{107}{3}\zeta_9\zeta_3 + \tfrac{47}{2}\zeta_7\zeta_5)\lambda^3 + (456\zeta_9\zeta_3 - 207\zeta_7\zeta_5 - 16\zeta_3^4)\lambda^2 + (-\tfrac{488}{3}\zeta_9\zeta_3 - 216\zeta_7\zeta_5)\lambda^3 + (456\zeta_9\zeta_3 - 207\zeta_7\zeta_5 - 16\zeta_3^4)\lambda^2 + (-\tfrac{488}{3}\zeta_9\zeta_3 - 216\zeta_7\zeta_5)\lambda^3 + (456\zeta_9\zeta_3 - 207\zeta_7\zeta_5 - 16\zeta_3^4)\lambda^2 + (-\tfrac{488}{3}\zeta_9\zeta_3 - 216\zeta_7\zeta_5)\lambda^3 + (456\zeta_9\zeta_3 - 207\zeta_7\zeta_5 - 16\zeta_3^4)\lambda^2 + (-\tfrac{488}{3}\zeta_9\zeta_3 - 216\zeta_7\zeta_5)\lambda^3 + (-\tfrac{488}{3}\zeta_9\zeta_9 - 216\zeta_7\zeta_7\zeta_5)\lambda^3 + (-\tfrac{488}{3}\zeta_9\zeta_9 - 216\zeta_7\zeta_7\zeta_7)\lambda^3 + (-\tfrac{488}{3}\zeta_9\zeta_9 - 216\zeta_7\zeta_
                                                                                                                               +\frac{272}{3}\zeta_3^4)\lambda + (\frac{1360}{3}\zeta_9\zeta_3 + 432\zeta_7\zeta_5 + \frac{32}{3}\zeta_3^4)
                                                                                  -\frac{7}{64}\zeta_{13}\lambda^5 + (-\frac{226501}{16800}\zeta_{13} + \zeta_7\zeta_3^2 - \frac{31}{10}\zeta_5^2\zeta_3 - \frac{157}{1400}\zeta_{5,3,5}^{\mathrm{sv}} + \frac{5}{56}\zeta_{3,7,3}^{\mathrm{sv}})\lambda^4 + (-\frac{1283839}{8400}\zeta_{13} + 34\zeta_7\zeta_3^2 + \frac{256}{5}\zeta_5^2\zeta_3)\lambda^4 + (-\frac{1283839}{16800}\zeta_{13} + 34\zeta_7\zeta_3^2 + \frac{256}{50}\zeta_5^2\zeta_3)\lambda^4 + (-\frac{1283839}{16800}\zeta_{13} + 34\zeta_7\zeta_3^2 + \frac{256}{50}\zeta_5^2\zeta_3)\lambda^4 + (-\frac{1283839}{16800}\zeta_{13} + 34\zeta_7\zeta_3^2 + \frac{256}{50}\zeta_3^2\zeta_3)\lambda^4 + (-\frac{1283839}{16800}\zeta_{13} + \frac{1283839}{16800}\zeta_{13} + \frac{1283839
                                                                                                                                      -\frac{549}{350}\zeta_{5,3,5}^{\text{sv}} + \frac{59}{28}\zeta_{3,7,3}^{\text{sv}})\lambda^3 + \left(-\frac{1447393}{1400}\zeta_{13} + 1236\zeta_7\zeta_3^2 - \frac{1128}{5}\zeta_5^2\zeta_3 - \frac{12339}{175}\zeta_{5,3,5}^{\text{sv}} + \frac{747}{14}\zeta_{3,7,3}^{\text{sv}}\right)\lambda^2
                                                                                                                               +(-618\zeta_{13}+336\zeta_7\zeta_3^2+336\zeta_5^2\zeta_3)\lambda+(1260\zeta_{13}+288\zeta_7\zeta_3^2+288\zeta_5^2\zeta_3)
14 \qquad (\frac{7}{16}\zeta_{11}\zeta_3+\zeta_9\zeta_5+\frac{9}{16}\zeta_7^2)\lambda^5+(\frac{10169}{240}\zeta_{11}\zeta_3+\frac{467}{8}\zeta_9\zeta_5+\frac{175}{16}\zeta_7^2-\frac{1}{5}\zeta_{3,5,3}^{\rm sv}\zeta_3)\lambda^4+(\frac{20381}{30}\zeta_{11}\zeta_3+\frac{1300}{9}\zeta_9\zeta_5+\frac{483}{4}\zeta_7^2)\lambda^2+(\frac{10169}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_{11}\zeta_3+\frac{1300}\zeta_{11}\zeta_3+\frac{1300}{240}\zeta_1+\frac{1300}{240}\zeta_1+\frac{1300}\zeta_1+\frac{1300}{24
                                                                                                                                   +40\zeta_5\zeta_3^3+\tfrac{28}{5}\zeta_{3,5,3}^{\mathrm{sv}}\zeta_3)\lambda^3+(\tfrac{32902}{5}\zeta_{11}\zeta_3-\tfrac{7306}{3}\zeta_9\zeta_5-\tfrac{3627}{2}\zeta_7^2+\tfrac{3664}{3}\zeta_5\zeta_3^3+\tfrac{1296}{5}\zeta_{3,5,3}^{\mathrm{sv}}\zeta_3)\lambda^2
                                                                                                                                   +(-664\zeta_{11}\zeta_3 - \frac{2824}{3}\zeta_9\zeta_5 - 540\zeta_7^2 + \frac{2752}{3}\zeta_5\zeta_3^3)\lambda + (1488\zeta_{11}\zeta_3 + 1360\zeta_9\zeta_5 + 648\zeta_7^2 + 128\zeta_5\zeta_3^3)
```

The results given in Table 1 confirm this conjecture for  $n \leq 14$ , and in [2] we give strong numerical evidence in its support also for n = 15 and n = 16. If true, Conjecture 1 would also explain the curious fact that when  $\mathcal{P}_N$  is normalized to have area  $\pi$  (as opposed to, say, normalizing  $\mathcal{P}_N$  to have circumradius 1), the low order coefficients of the resulting asymptotic expansion do not involve even zeta values (see [4, p. 125]).

By analyzing the general recursion for  $C_n(\lambda)$  obtained in the proof of Theorem 1 we obtain a formula for the generating function of the first two coefficients of the polynomials  $C_n(\lambda)$ .

**Theorem 2.** The coefficients  $C_n(0)$  and  $C'_n(0)$  satisfy the generating series identity

$$\sum_{n\geq 0} (C_n(0) + C'_n(0)\lambda)z^n = \frac{\Gamma(1+z)^2\Gamma(1-2z)}{\Gamma(1-z)^2\Gamma(1+2z)} \left(1 - \frac{\lambda}{2} \sum_{n\geq 1} \frac{(2z)_n^2 z^3}{n!^2 (z+n)^3}\right),\tag{4}$$

where  $(x)_n = x(x+1) \dots (x+n-1)$  denotes the rising Pochhammer symbol.

Using this formula we also prove the following.

**Theorem 3.** The coefficients  $C_n(0)$  and  $C'_n(0)$  are polynomials with rational coefficients in odd zeta values of homogeneous weight n.

The proof is based on a hypergeometric identity (27) of Ramanujan-Dougall type that could be of independent interest. Theorem 3 confirms Conjecture 1 for the first two coefficients  $C_n(0)$  and  $C'_n(0)$ . Note that the expression for  $C_{11}$  from Table 1 shows that  $C''_{11}(0)$  involves  $\zeta_{3,5,3}^{\text{sv}}$ , and thus the claim of Theorem 3 in general fails for  $C''_n(0)$ , assuming the (widely believed) algebraic independence of  $\zeta_{3,5,3}^{\text{sv}}$  and  $\zeta(2m+1)$ ,  $m \geq 1$  (see [6, p. 35]).

As a final remark, we note that the normalizing factor

$$\frac{\Gamma(1+z)^2\Gamma(1-2z)}{\Gamma(1-z)^2\Gamma(1+2z)}$$

that appears in several of our formulas is a specialization of Virasoro's closed bosonic string amplitude [24]. We do not know if this is a simple coincidence, or if there is some conceptual explanation for this.

### 2. Multiple polylogarithms and multiple zeta values

In this section we very briefly recall some basic properties of multiple polylogarithms and multiple zeta values. For a much more detailed introduction (including the algebraic structure and interpretation of MZVs as periods of mixed Tate motives) we refer the reader to [25], [7].

Let  $m_1, \ldots, m_r$  be positive integers. The one-variable multiple polylogarithm  $\text{Li}_{m_1,\ldots,m_r}(z)$  is an analytic function defined by the power series

$$\operatorname{Li}_{m_1,\dots,m_r}(z) := \sum_{\substack{0 < n_1 < n_2 < \dots < n_r \\ 1}} \frac{z^{n_r}}{n_1^{m_1} n_2^{m_2} \dots n_r^{m_r}}, \qquad |z| < 1.$$
 (5)

For  $m_r > 1$  the above series converges absolutely for  $|z| \leq 1$  and we define

$$\zeta(m_1, \dots, m_r) := \sum_{0 < n_1 < n_2 < \dots < n_r} \frac{1}{n_1^{m_1} n_2^{m_2} \dots n_r^{m_r}} = \operatorname{Li}_{m_1, \dots, m_r}(1).$$
 (6)

The numbers  $\zeta(m_1,\ldots,m_r)$  are called multiple zeta values (MZVs). We denote by  $\mathfrak{Z}$  the  $\mathbb{Q}$ -linear span of all multiple zeta values of weight k, i.e., the linear span of  $\zeta(m_1,\ldots,m_r)$  over all r-tuples  $(m_1,\ldots,m_r)$  satisfying  $m_1+\cdots+m_r=k$ . The  $\mathbb{Q}$ -vector space  $\mathfrak{Z}$  forms an algebra (see (9) below), and multiplication respects weight, i.e.,  $\mathfrak{Z}_k \cdot \mathfrak{Z}_l \subseteq \mathfrak{Z}_{k+l}$ . Zagier [27] has conjectured that there are no rational linear relations between elements of  $\mathfrak{Z}_k$  for different k (that is, that  $\mathfrak{Z}=\bigoplus_{k>0}\mathfrak{Z}_k$ ) and that dim  $\mathfrak{Z}_k=d_k$ , where  $d_k$  are defined by the generating series

$$\frac{1}{1 - x^2 - x^3} = \sum_{k > 0} d_k x^k \,.$$

The upper bound dim  $\mathfrak{Z}_k \leq d_k$  has been proved independently by Goncharov and Terasoma, but no nontrivial lower bounds for dim  $\mathfrak{Z}_k$  are presently known.

For our purposes it is more convenient to index multiple polylogarithms by words in two letters  $X = \{x_0, x_1\}$ , reflecting their structure as iterated integrals as opposed to the definition as an infinite sum (5). In our treatment we mainly follow Brown [5] (see also [13]). Let  $X^{\times}$  be the free noncommutative monoid generated by X, i.e., the set of all words in  $x_0, x_1$  equipped with the concatenation product. Then  $\{\text{Li}_w\}_{w \in X^{\times}}$  is a family of analytic functions on the cut plane  $\mathbb{C} \setminus ((-\infty, 0] \cup [1, \infty))$  defined by the recursive relations

$$\frac{d}{dz}\operatorname{Li}_{x_0w}(z) = \frac{\operatorname{Li}_w(z)}{z}, \qquad \frac{d}{dz}\operatorname{Li}_{x_1w}(z) = \frac{\operatorname{Li}_w(z)}{1-z}, \qquad w \in X^{\times}$$
(7)

together with the following initial conditions:  $\operatorname{Li}_e(z) = 1$ ,  $\operatorname{Li}_{x_0^n}(z) = \frac{1}{n!} \log^n(z)$ , and  $\lim_{z \to 0} \operatorname{Li}_w(z) = 0$  for all  $w \in X^{\times}$  not of the form  $x_0^n$ . Here  $e \in X^{\times}$  denotes the empty word. These conditions uniquely determine  $\operatorname{Li}_w(z)$  and for  $m_1, \ldots, m_r \ge 1$  one has

$$\operatorname{Li}_{x_0^{m_r-1}x_1...x_0^{m_1-1}x_1}(z) = \operatorname{Li}_{m_1,...,m_r}(z). \tag{8}$$

We also extend the notation  $\text{Li}_w(z)$  by linearity to the elements of the monoid ring  $\mathbb{C}\langle X \rangle$ , i.e., for any formal combination  $\sum_i a_i w_i$  we set  $\text{Li}_{\sum_i a_i w_i}(z) = \sum_i a_i \text{Li}_{w_i}(z)$ . Note that the algebra  $\mathbb{C}\langle X \rangle$  is graded by word length, and we denote by  $\mathbb{C}\langle X \rangle_n$  the *n*-the graded piece. We will also write |w| for the length of  $w \in X^{\times}$ 

and we will say that the function  $\text{Li}_w(z)$  has weight |w|. (Since the functions  $\text{Li}_w(z)$  are linearly independent over  $\mathbb{C}(z)$ , see [5], this notion of weight is well-defined.)

An important property of the space of multiple polylogarithms is that it is closed under multiplication. More precisely, one has

$$\operatorname{Li}_{w}(z)\operatorname{Li}_{w'}(z) = \operatorname{Li}_{w \sqcup w'}(z). \tag{9}$$

Here  $\mathbf{u} \colon \mathbb{C}\langle X \rangle \times \mathbb{C}\langle X \rangle \to \mathbb{C}\langle X \rangle$  denotes the shuffle product, defined on words by

$$a_1 \dots a_k \coprod a_{k+1} \dots a_{k+l} = \sum_{\sigma} a_{\sigma(1)} \dots a_{\sigma(k+l)}$$

where  $\sigma$  runs over all permutations satisfying  $\sigma^{-1}(1) < \cdots < \sigma^{-1}(k)$  and  $\sigma^{-1}(k+1) < \cdots < \sigma^{-1}(k+l)$ .

Note that for  $w \in X^{\times} x_1$  the function  $\text{Li}_w(z)$  extends analytically to  $\mathbb{C} \setminus [1, \infty)$ , and for  $w \in x_0 X^{\times} x_1$  it is moreover continuous on  $\overline{\mathbb{D}}$ . We will call the words  $w \in x_0 X^{\times} x_1$  convergent and we will also call convergent any formal linear combination of convergent words in  $\mathbb{C}\langle X\rangle$  (in other words, all elements of  $x_0\mathbb{C}\langle X\rangle x_1$  are called convergent). An important corollary of (9) is that for any  $w \in X^{\times} x_1$  there exists a unique collection of convergent elements  $w_0, w_1, \ldots, w_k \in \mathbb{Q}\langle X\rangle$  such that

$$\operatorname{Li}_{w}(z) = \operatorname{Li}_{w_{0}}(z) + \operatorname{Li}_{w_{1}}(z)\operatorname{Li}_{1}(z) + \dots + \operatorname{Li}_{w_{k}}(z)\operatorname{Li}_{1}^{k}(z).$$

The function  $\text{Li}_1(z)$  is simply  $-\log(1-z)$ . The above decomposition allows one to extend the definition of multiple zeta values  $\zeta(w) = \text{Li}_w(1)$  to cases when the series diverges by setting  $\text{Li}_w(1) := \text{Li}_{w_0}(1)$  for all  $w \in X^{\times} x_1$ .

In the proof of our main result we will use several identities involving multiple polylogarithms. First, let us note the following simple corollaries of the definition of  $\text{Li}_w$ .

**Lemma 1.** For all  $w \in X^{\times} x_1$  and  $k \geq 0$  we have

$$\operatorname{Li}_{x_0^{k+1}w}(z) = \frac{1}{k!} \int_0^z \operatorname{Li}_w(t) \log^k(z/t) \frac{dt}{t}, \qquad z \in \overline{\mathbb{D}}.$$

**Proof.** This follows trivially from (7) by induction on k.  $\square$ 

**Lemma 2.** For all  $w \in X^{\times} x_1$  we have

$$\int_{0}^{1} \operatorname{Li}_{w}(e^{2\pi i t}) dt = 0.$$

**Proof.** This follows from  $\operatorname{Li}_w(e^{2\pi it}) = \frac{1}{2\pi i} \frac{d}{dt} \operatorname{Li}_{x_0 w}(e^{2\pi it})$ .  $\square$ 

Our proof of Theorem 1 is based on the following result.

**Proposition 1.** Let  $u, v \in X^{\times} x_1$  and let k = |u| + |v|. Then there exist elements  $\alpha(u, v)$  and  $\beta(u, v)$  in  $\bigoplus_{j=0}^{k-1} \mathfrak{Z}_j \otimes \mathbb{Q}\langle X \rangle_{k-j-1} x_1$  and  $A_{u,v} \in \mathfrak{Z}_k$  such that

$$\operatorname{Li}_{u}(z)\operatorname{Li}_{v}(z^{-1}) = A_{u,v} + \operatorname{Li}_{\alpha(u,v)}(z) + \operatorname{Li}_{\beta(u,v)}(z^{-1}), \qquad z \in \mathbb{C} \setminus [0,+\infty).$$
(10)

Moreover, if u and v are convergent, then  $\alpha(u,v)$  and  $\beta(u,v)$  are also convergent.

**Proof.** We will prove the statement by induction on k for all  $u, v \in X^{\times} x_1 \sqcup \{e\}$ . For the base of induction, when either u = e or v = e the identity becomes trivial if we set  $A_{u,e} = A_{e,v} = 0$ ,  $\alpha(u,e) = u$ ,  $\alpha(e,v) = 0$ , and  $\beta(u,e) = 0$ ,  $\beta(e,v) = v$ .

Note that from (7) it follows that for all  $w \in X^{\times}$  we have

$$\frac{d}{dz} \operatorname{Li}_{x_0 w}(z^{-1}) = -\frac{1}{z} \operatorname{Li}_w(z^{-1}), \qquad \frac{d}{dz} \operatorname{Li}_{x_1 w}(z^{-1}) = (\frac{1}{z} + \frac{1}{1-z}) \operatorname{Li}_w(z^{-1}). \tag{11}$$

Therefore, if we set

$$F_{u,v}(z) = \operatorname{Li}_u(z)\operatorname{Li}_v(z^{-1}),$$

then for any  $a, b \in X$ ,  $u, v \in X^{\times}$  we have

$$\frac{d}{dz}F_{au,bv}(z) = \varphi_a(z)F_{u,bv}(z) + \psi_b(z)F_{au,v}(z)$$

$$= \varphi_a(z)(A_{u,bv} + \operatorname{Li}_{\alpha(u,bv)}(z) + \operatorname{Li}_{\beta(u,bv)}(\frac{1}{z})) + \psi_b(z)(A_{au,v} + \operatorname{Li}_{\alpha(au,v)}(z) + \operatorname{Li}_{\beta(au,v)}(\frac{1}{z})),$$

where  $\varphi_{x_0}(z) = \frac{1}{z}$ ,  $\varphi_{x_1}(z) = \frac{1}{1-z}$ ,  $\psi_{x_0}(z) = -\frac{1}{z}$ , and  $\psi_{x_1}(z) = \frac{1}{z} + \frac{1}{1-z}$ . In view of this we recursively define

$$\alpha(au, bv) = a\alpha(u, bv) + \tilde{b}\alpha(au, v) + (A_{u,bv}\delta(a) + A_{au,v}\frac{1 - \delta(b)}{2})x_1$$
  

$$\beta(au, bv) = \tilde{a}\beta(u, bv) + b\beta(au, v) + (A_{au,v}\delta(b) + A_{u,bv}\frac{1 - \delta(a)}{2})x_1,$$
(12)

where  $\widetilde{x_0} = -x_0$ ,  $\widetilde{x_1} = x_0 + x_1$ , and  $\delta$  is defined by  $\delta(x_1) = 1$ ,  $\delta(x_0) = -1$ . Then by induction we obtain that

$$\mathrm{Li}_u(z)\mathrm{Li}_v(z^{-1})-\mathrm{Li}_{\alpha(u,v)}(z)-\mathrm{Li}_{\beta(u,v)}(z^{-1})=\mathrm{const}=:A_{u,v}\,.$$

If  $u, v, \alpha$ , and  $\beta$  are all convergent, then we may simply take z = 1 to get  $A_{u,v} = \text{Li}_u(1)\text{Li}_v(1) - \text{Li}_{\alpha(u,v)}(1) - \text{Li}_{\beta(u,v)}(1)$ . Otherwise we take  $z = e^{2\pi ix}$  and take the limit  $x \to 0+$ , which corresponds to a regularization of  $\text{Li}_v(1)$  given by

$$\operatorname{Li}_{w}(e^{\pm 2\pi i0}) := \sum_{j=0}^{k} \operatorname{Li}_{w_{j}}(1)(\pm \frac{\pi i}{2})^{j},$$

where  $\text{Li}_w(z) = \sum_{j=0}^k \text{Li}_{w_j}(z) \text{Li}_1^j(z)$  with all  $w_j$  in  $x_0 \mathbb{C}\langle X \rangle x_1$ . Thus  $A_{u,v} \in \mathfrak{Z}_k$  and by induction we get also that  $\alpha(u,v)$  and  $\beta(u,v)$  belong to  $\bigoplus_{j=0}^{k-1} \mathfrak{Z}_j \otimes \mathbb{Q}\langle X \rangle_{k-j-1} x_1$ .

To verify the last claim let us consider  $u = x_0 u'$ ,  $v = x_0 v'$ . The recursive definition (12) with  $a = b = x_0$  shows that  $\alpha(u, v)$  and  $\beta(u, v)$  would be convergent if we can show that  $A_{u', x_0 v'} = A_{x_0 u', v'}$ . But the calculation of the derivative of  $F_{u,v}$  shows that

$$i\frac{d}{dt}F_{u,v}(e^{it}) = A_{u',x_0v'} - A_{x_0u',v'} + \text{Li}_w(e^{it}) + \text{Li}_{w'}(e^{-it})$$

for some  $w, w' \in \mathbb{C}\langle X \rangle x_1$  and hence, by Lemma 2, we obtain  $A_{u',x_0v'} = A_{x_0u',v'}$ .  $\square$ 

Remark 1. The proof shows that we may take  $\beta(u,v) = \alpha(v,u)$ . Note also that if we extend the definition of  $\alpha(u,v)$ ,  $\beta(u,v)$ , and  $A_{u,v}$  to bilinear functionals on  $\mathbb{C}\langle X\rangle x_1 \times \mathbb{C}\langle X\rangle x_1$ , the identity (10) remains true for all  $u,v\in\mathbb{C}\langle X\rangle x_1$ .

As a corollary of the above proposition we have the following curious fact.

Corollary 1. For all  $u, v \in X^{\times} x_1$  we have

$$\int_{0}^{1} \operatorname{Li}_{u}(e^{2\pi i t}) \operatorname{Li}_{v}(e^{-2\pi i t}) dt \in \mathfrak{Z}_{|u|+|v|}.$$

**Proof.** It follows from (10) and Lemma 2 that

$$A_{u,v} = \int_{0}^{1} \operatorname{Li}_{u}(e^{2\pi it}) \operatorname{Li}_{v}(e^{-2\pi it}) dt,$$

and the claim then follows from Proposition 1.  $\Box$ 

As a further corollary, note that when u and v are both convergent equation (10) implies

$$\operatorname{Re} \operatorname{Li}_{u}(z)\operatorname{Li}_{v}(\overline{z}) = A_{u,v} + \operatorname{Re} \operatorname{Li}_{\alpha(u,v)+\beta(u,v)}(z), \qquad |z| = 1.$$

This formula thus gives a purely algebraic solution of the Dirichlet boundary value problem  $u(z) = \varphi(z)$  for |z| = 1 where  $\varphi$  is of the form  $\varphi(z) = \text{Re Li}_u(z) \text{Li}_v(\overline{z})$  and u is sought to be harmonic in  $\mathbb{D}$ . It is exactly in this form that we will use Proposition 1 in the proof of Theorem 1.

#### 3. Proof of Theorem 1

Let us fix the polygon  $\mathcal{P}_N \subset \mathbb{C}$  to be the convex hull of  $\{c\zeta^j\}_{0 \leq j < N}$ , where  $\zeta$  is a primitive n-th root of unity, and c > 0 is chosen so that  $\operatorname{Area}(\mathcal{P}_N) = \pi$ . We will utilize the classical Schwarz-Christoffel map,  $f \colon \mathbb{D} \to \mathcal{P}_N$ , which maps the unit disk  $\mathbb{D}$  conformally onto  $\mathcal{P}_N$ . It is given by any of the following equivalent expressions

$$f(z) = c_N z_2 F_1\left(\frac{2}{N}, \frac{1}{N}, 1 + \frac{1}{N}; z^N\right) = c_N \int_0^z \frac{d\zeta}{(1 - \zeta^N)^{2/N}}$$
(13)

where the constant

$$c_N = \sqrt{\frac{\Gamma(1 - 1/N)^2 \Gamma(1 + 2/N)}{\Gamma(1 + 1/N)^2 \Gamma(1 - 2/N)}}$$
(14)

is determined by the condition that  $Area(\mathcal{P}_N) = \pi$ . Here  ${}_2F_1$  is the ordinary Gauss hypergeometric function

$$_{2}F_{1}(a,b,c;z) = \sum_{n\geq 0} \frac{(a)_{n}(b)_{n}}{(c)_{n}} \frac{z^{n}}{n!}, \qquad |z| < 1,$$

where  $(x)_n := x(x+1) \dots (x+n-1)$  denotes the rising Pochhammer symbol.

The first fact that we will need is that the function  $F_N(x) := {}_2F_1(2/N, 1/N, 1+1/N; x)$  can be expanded as a power series in 1/N (convergent for  $N \ge 3$ ) whose coefficients are multiple polylogarithms. Let us recall the definition of Nielsen polylogarithms (see [16], [9])

$$S_{n,p}(z) = \frac{(-1)^{n+p-1}}{(n-1)!p!} \int_{0}^{1} \log^{n-1}(t) \log^{p}(1-zt) \frac{dt}{t} = \operatorname{Li}_{1,\dots,1,n+1}(z) = \operatorname{Li}_{x_{0}^{n} x_{1}^{p}}(z).$$
 (15)

**Lemma 3.** For all  $N \geq 3$  and  $|x| \leq 1$  we have

$$_{2}F_{1}\left(\frac{2}{N}, \frac{1}{N}, 1 + \frac{1}{N}; x\right) = 1 + \sum_{n=2}^{\infty} S_{n}(x)N^{-n},$$
 (16)

where

$$S_n(x) = \sum_{j=1}^{n-1} (-1)^{j-1} 2^{n-j} S_{j,n-j}(x).$$

**Proof.** This follows by expanding in powers of 1/N the right hand side of

$$_{2}F_{1}\left(\frac{2}{N},\frac{1}{N},1+\frac{1}{N};x\right)=1+\frac{1}{N}\int_{0}^{1}t^{1/N}((1-tx)^{-2/N}-1)\frac{dt}{t}$$

and using the definition (15).  $\Box$ 

We will also need a formula for the asymptotic expansion of the Bessel function  $J_0(x)$  around its zero. Recall that  $J_0(x)$  satisfies  $xJ_0''(x) + J_0'(x) + xJ_0(x) = 0$  and can be defined by the Taylor series

$$J_0(x) = \sum_{n>0} \frac{\left(-\frac{x^2}{4}\right)^n}{n!^2} \,.$$

**Proposition 2.** (i) For  $n \geq 0$  define

$$E_n(x) := \sum_{j=0}^n \frac{e^{2jx}(x + H_{n-j} - H_j)}{j!^2(n-j)!^2},$$

where  $H_n = \sum_{j=1}^n \frac{1}{j}$ ,  $H_0 = 0$ . Then  $E_n(x) = O(x^{2n+1})$ ,  $x \to 0$ . (ii) Let  $\alpha$  be a zero of  $J_0(x)$ . Then

$$-\frac{J_0(\alpha e^x)}{\alpha J_1(\alpha)} = \sum_{n>0} (-\frac{\alpha^2}{4})^n E_n(x). \tag{17}$$

**Proof.** (i) Define  $W_n$  by

$$W_n(x) := \int_0^\infty E_n(xt)e^{-t}dt = \sum_{j=0}^n \frac{1}{j!^2(n-j)!^2} \left( \frac{x}{(1-2jx)^2} + \frac{H_{n-j} - H_j}{1-2jx} \right).$$

Note that if  $E_n(x) = \sum_m a_m x^m$ , then  $W_n(x) = \sum_m m! a_m x^m$ , so it suffices to show that  $W_n(x) = O(x^{2n+1})$ ,  $x \to 0$ . We claim that

$$W_n(x) = \frac{4^n x^{2n+1}}{\prod_{j=1}^n (1-2jx)^2},$$

which clearly implies  $W_n(x) = O(x^{2n+1})$ . Let  $R_n(x)$  denote the difference between the left hand side and the right hand side in the above equation. A simple calculation shows that  $R_n(x) \to 0$  as  $x \to \infty$ , and

since  $R_n \in \mathbb{Q}(x)$ , it is enough to show that it has no poles. The only potential singularities are at  $x = \frac{1}{2k}$ ,  $1 \le k \le n$ . If we let  $x = \frac{1}{2k} - \varepsilon$ , then

$$n!^2 R_n(x) = \binom{n}{k}^2 \left( \frac{\frac{1}{2k} - \varepsilon}{(2k\varepsilon)^2} + \frac{H_{n-k} - H_k}{2k\varepsilon} \right) - \frac{\varepsilon^{-2} (\frac{1}{2k} - \varepsilon)^{2n+1}}{\prod_{i \neq k} (\frac{1}{2i} - \frac{1}{2k} + \varepsilon)^2} + O(1), \qquad \varepsilon \to 0.$$

(Here  $\prod_{j\neq k}$  denotes the product over  $1\leq j\leq n,\ j\neq k$ .) Then the coefficient in front  $\varepsilon^{-2}$  vanishes since  $\binom{n}{k}^2=\prod_{j\neq k}(\frac{k}{j}-1)^{-2}$ , and for  $\varepsilon^{-1}$  the vanishing is equivalent to

$$1 - 2k(H_{n-k} - H_k) = (2n+1) + \sum_{\substack{1 \le j \le n \\ j \ne k}} \frac{2j}{k-j},$$

which is again easy to verify.

(ii) Let us denote the left hand side of (17) by f(x) and the right hand side by g(x). From the differential equation  $xJ_0''(x) + J_0'(x) + xJ_0(x)$  together with  $J_0'(x) = -J_1(x)$ , we obtain that  $f''(x) + \alpha^2 e^{2x} f(x) = 0$  and f(0) = 0, f'(0) = 1. Thus, it is enough to check that g(x) satisfies the same differential equation and initial conditions. The conditions g(0) = 0, g'(0) = 1 follow from part (i). Using the easily checked identity

$$\frac{e^{2jx}j^2(x+H_{n+1-j}-H_j)+e^{2jx}j}{j!^2(n+1-j)!^2} = \frac{e^{2jx}j^2(x+H_{n-j+1}-H_{j-1})}{(j-1)!^2(n-j+1)!^2}, \qquad 1 \le j \le n+1$$

we get that  $g''(x) + \alpha^2 e^{2x} g(x)$ .  $\square$ 

Finally, to prove the asymptotic expansion we will employ the following version of the "method of particular solutions".

**Proposition 3.** Let  $\Omega$  be a bounded domain in  $\mathbb{R}^2$ , and let  $f \colon \overline{\Omega} \to \mathbb{R}$  be a function in  $C^2(\Omega) \cap C(\overline{\Omega})$  that satisfies  $\Delta f + \lambda' f = 0$  in  $\Omega$ ,  $\frac{1}{|\Omega|} \int_{\Omega} |f(x)|^2 dx = 1$ , and  $\sup_{x \in \partial \Omega} |f(x)| \leq \varepsilon$ , where  $\varepsilon < 1$ . Then there exists a Dirichlet eigenvalue  $\lambda$  of  $\Omega$  such that  $|\lambda' - \lambda| \leq \lambda \varepsilon$ .

**Proof.** This is a special case of [18, Theorem 1].  $\square$ 

We are now ready to prove our main result.

**Proof of Theorem 1.** To simplify notation we set  $\lambda^{(N)} := \lambda_k(\mathcal{P}_N)$  and  $\lambda := \lambda_k(\mathbb{D})$ . Since the  $\lambda$ -eigenfunction of  $\mathbb{D}$  is radially-symmetric, we may assume that, for all sufficiently large N, the  $\lambda^{(N)}$ -eigenfunction of  $\mathcal{P}_N$  is dihedrally-symmetric. More precisely, if

$$\begin{cases} \Delta \varphi(z) + \lambda^{(N)} \varphi(z) = 0, \\ \varphi(z) = 0, \quad z \in \partial \mathcal{P}_N, \end{cases}$$
(18)

then we may assume that  $\varphi(e^{2\pi i/N}z) = \varphi(\overline{z}) = \varphi(z)$ .

By the general theory developed by Vekua [23, (13.5), p. 58] any function  $\varphi$  that satisfies  $\Delta \varphi + \lambda^{(N)} \varphi = 0$  in  $\mathcal{P}_N$  can be represented as

$$\varphi(z) = a_0 J_0(\sqrt{\lambda^{(N)}}|z|) + \operatorname{Re} \int_0^z U(t) J_0\left(\sqrt{\lambda^{(N)}\overline{z}(z-t)}\right) dt, \qquad (19)$$

where  $a_0 \in \mathbb{R}$  and  $U: \mathcal{P}_N \to \mathbb{C}$  is some holomorphic function. Since by assumption  $\varphi(z)$  is dihedrally-symmetric, we may write  $U(f(t)) = \widetilde{U}(t^N)/t$ , where  $\widetilde{U}(0) = 0$  and the Taylor series of  $\widetilde{U}$  at 0 has real coefficients (we recall that f is defined by (13)). Then

$$\varphi(f(z)) = a_0 J_0(\sqrt{\lambda^{(N)}}|f(z)|) + \operatorname{Re} \int_0^z f'(t) U(f(t)) J_0\left(\sqrt{\lambda^{(N)}}\overline{f(z)}(f(z) - f(t))\right) dt$$

$$= a_0 J_0(\sqrt{\lambda^{(N)}}|f(z)|) + c_N \operatorname{Re} \int_0^z (1 - t^N)^{-2/N} \widetilde{U}(t^N) J_0\left(\sqrt{\lambda^{(N)}}\overline{f(z)}(f(z) - f(t))\right) \frac{dt}{t}.$$

After replacing z and t by  $z^{1/N}$  and  $t^{1/N}$  respectively and setting  $\psi(z) \coloneqq \varphi(f(z^{1/N}))$  and  $V(z) \coloneqq \frac{\tilde{U}(z)}{(1-z)^{2/N}}$  we obtain

$$\psi(z) = a_0 J_0(\rho^{1/2}|z|^{1/N}|F_N(z)|) + \frac{c_N}{N} \operatorname{Re} \int_0^z V(t) K(z, t) \frac{dt}{t},$$
(20)

where we set  $\rho := c_N^2 \lambda^{(N)}$  and

$$K(z,t) := J_0 \left( \rho^{1/2} |z|^{1/N} \sqrt{F_N(\overline{z}) (F_N(z) - (t/z)^{1/N} F_N(t))} \right).$$

Now we make an ansatz that

$$\rho \sim \lambda \exp\left(\frac{\kappa_1}{N} + \frac{\kappa_2}{N^2} + \dots\right),$$

$$V(z) \sim V_0(z) + \frac{V_1(z)}{N} + \frac{V_2(z)}{N^2} + \dots,$$
(21)

where  $V_i : \mathbb{D} \to \mathbb{C}$  are holomorphic and  $V_i(0) = 0$ .

In view of Proposition 2 (ii) it is convenient to set  $a_0 = \frac{c_N}{\lambda^{1/2}J_1(\lambda^{1/2})}$ . We will expand (20) as an asymptotic series in powers of 1/N and then recursively compute  $\kappa_j$  and  $V_j$  using the boundary condition  $\psi(z) = 0$ , |z| = 1. Note that by (16)  $F_N(x) = 1 + O(N^{-2})$  and using (16) and the expansion  $(t/z)^{1/N} = \sum_{n\geq 0} \frac{\log^n(t/z)}{n!} N^{-n}$  we get

$$\begin{split} K(z,t) &= \sum_{n=0}^{r} (-\frac{\rho}{4})^n \frac{F_N(\overline{z})^n (F_N(z) - (t/z)^{1/N} F_N(t))^n}{n!^2} + O(N^{-r-1}) \\ &= \sum_{u,v,w,m} \gamma_{u,v,w,m} \mathrm{Li}_u(\overline{z}) \mathrm{Li}_v(z) \mathrm{Li}_w(t) \log^m(z/t) N^{-|u|-|v|-|w|-m} + O(N^{-r-1}) \,, \end{split}$$

where  $\gamma_{u,v,w,m}$  are coefficients that depend on  $\kappa_i$  and the summation is over words  $u,v,w \in x_0 X^{\times} x_1$  and  $m \geq 0$  satisfying  $|u| + |v| + |w| + m \leq r$ . We get a similar expression (involving only products  $\text{Li}_u(z)\text{Li}_v(\overline{z})$ ) after expanding  $a_0 J_0(\rho^{1/2}|F_N(z)|)$  using (17).

We claim that  $\kappa_i$  and  $V_i(z)$  can be calculated inductively by comparing the coefficients of the 1/N-expansion. Indeed, comparing the coefficients of 1/N we see that

$$\frac{\kappa_1}{2} - \text{Re} \int_0^z V_0(t) \frac{dt}{t} = 0, \qquad |z| = 1,$$

Table 2 The functions  $V_n(z)$  for  $n \leq 4$ .

n	$V_n(z)$
0	0
1	$2 \mathrm{Li}_1(z)$
2	$(\frac{\lambda}{2}-2)\mathrm{Li}_2(z)+4\mathrm{Li}_{1,1}(z)$
3	$(\frac{\lambda^2}{16} - \lambda + 2) \text{Li}_3(z) + (3\lambda - 12) \text{Li}_{1,2}(z) + (\lambda - 4) \text{Li}_{2,1}(z) + 2^3 \text{Li}_{1,1,1}(z)$
4	$(\frac{\lambda^3}{192} - \frac{\lambda^2}{8} - \frac{\lambda}{2} - 2) \text{Li}_4(z) + (\frac{\lambda^2}{8} - 2\lambda + 4) \text{Li}_{3,1}(z) + (\frac{\lambda^2}{4} - 4\lambda + 12) \text{Li}_{2,2}(z)$
	+ $(\frac{5\lambda^2}{8} - 8\lambda + 28)$ Li <sub>1,3</sub> $(z)$ + $(2\lambda - 8)$ Li <sub>2,1,1</sub> $(z)$ + $(6\lambda - 24)$ Li <sub>1,2,1</sub> $(z)$
	+ $(14\lambda - 56)$ Li <sub>1,1,2</sub> $(z) + 2^4$ Li <sub>1,1,1,1</sub> $(z) + 2\zeta_3$ Li <sub>1</sub> $(z)$

so that  $\kappa_1 = V_0(z) = 0$ . In general, assume that  $\kappa_i \in \mathfrak{Z}_i[\lambda]$  and  $V_{i-1}(z) = \operatorname{Li}_{v_{i-1}}(z)$  for  $i = 1, \ldots, k$ , where  $v_i \in \mathfrak{Z}[\lambda]\langle X\rangle x_1$  is of total weight i (we define the total weight of  $\lambda^a zw$ , where  $z \in \mathfrak{Z}_k$  to be k + |w|). Note that by Lemma 1

$$\int_{0}^{z} \operatorname{Li}_{u}(\overline{z}) \operatorname{Li}_{v}(z) \operatorname{Li}_{w}(t) \log^{m}(z/t) \frac{dt}{t} = m! \operatorname{Li}_{u}(\overline{z}) \operatorname{Li}_{w'}(z),$$

where  $w' = v \coprod x_0^{m+1} w$ . Thus, when comparing the coefficients of  $N^{-k-1}$ , we need to ensure an identity of the form

$$\frac{\kappa_{k+1}}{2} - \operatorname{Re} \int_{0}^{z} V_{k}(t) \frac{dt}{t} - \sum_{u,v} \gamma_{u,v} \operatorname{Re} \operatorname{Li}_{u}(z) \operatorname{Li}_{v}(\overline{z}) = 0, \qquad |z| = 1,$$

where the terms in the sum only depend on already computed quantities  $\kappa_1, \ldots, \kappa_k$  and  $V_0(z), \ldots, V_{k-1}(z)$  and all have total weight k+1 (where we define the total weight of  $\gamma \operatorname{Li}_u(z) \operatorname{Li}_v(\overline{z})$  for  $\gamma \in \mathfrak{Z}_k[\lambda]$  to be |u|+|v|+k). By Proposition 1 this amounts to setting

$$x_0 v_k = -\sum_{u,v} \gamma_{u,v} (\alpha(u,v) + \beta(u,v)),$$
  
$$\frac{\kappa_{k+1}}{2} = \sum_{u,v} \gamma_{u,v} A_{u,v}.$$

This indeed can be done since by assumption the elements u and v are convergent and hence  $\alpha(u,v), \beta(u,v) \in x_0\mathbb{C}\langle X\rangle x_1$ . This gives an explicit algebraic recursion for  $\kappa_n$  and  $V_n(z)$  that shows, in particular, that  $\kappa_n \in \mathfrak{Z}_n[\lambda]$ . In Table 2 we list the functions  $V_n(z)$  for  $n \leq 4$ . We also note that the coefficients  $\kappa_n$  vanish for  $n \leq 4$ .

We still need to verify that the ansatz (21) indeed gives an asymptotic expansion for  $\lambda^{(N)}$ . To see this, note that plugging a truncated solution for the boundary condition  $\psi(z) = 0$ , |z| = 1 back into (19) we obtain a sequence of functions  $\varphi^{N,r} \colon \mathcal{P}_N \to \mathbb{R}$ , and numbers  $\lambda^{N,r}$ . The numbers  $\lambda^{N,r}$  converge to  $\lambda_k$  as  $N \to \infty$  for each fixed r and the functions  $\varphi^{N,r}$  satisfy

$$\Delta \varphi^{N,r}(z) + \lambda^{N,r} \varphi^{N,r}(z) = 0, \qquad z \in \mathcal{P}_N,$$

together with  $\|\varphi^{N,r}\|_2 \gg 1$  and  $\|\varphi^{N,r}|_{\partial \mathcal{P}_N}\|_{\infty} \ll_r N^{-r-1}$ . Therefore, applying Proposition 3 shows that  $|\lambda^{N,r} - \lambda_k(\mathcal{P}_N)| \ll_r N^{-r-1}$ , so that  $\lambda^{N,r}$  indeed give an asymptotic expansion for  $\lambda_k(\mathcal{P}_N)$ .

Finally, the coefficients  $C_n(\lambda)$  are related to  $\kappa_n(\lambda)$  by the generating series identity

$$\exp\left(\kappa_1(\lambda)z + \kappa_2(\lambda)z^2 + \dots\right) = \frac{\Gamma(1-z)^2\Gamma(1+2z)}{\Gamma(1+z)^2\Gamma(1-2z)} \left(1 + \sum_{n\geq 1} C_n(\lambda)z^n\right),\,$$

and using

$$\frac{\Gamma^2(1+z)\Gamma(1-2z)}{\Gamma^2(1-z)\Gamma(1+2z)} = \exp\left(\sum_{k>1} \zeta(2k+1) \frac{4(4^k-1)z^{2k+1}}{2k+1}\right)$$
(22)

we obtain that  $C_n \in \mathfrak{Z}_n[\lambda]$ .  $\square$ 

# 4. Explicit formulas for $C_n(0)$ and $C'_n(0)$

**Proof of Theorem 2.** We follow the algebraic recursion for  $\kappa_k$  and  $V_k(z)$  given in the proof of Theorem 1 ignoring all the terms involving  $\lambda^k$  for  $k \geq 2$  (in other words we work modulo the ideal generated by  $\lambda^2$ ). For this we write

$$V(z) = V^{(0)}(z) + \lambda V^{(1)}(z) + O(\lambda^2)$$

and

$$\kappa\coloneqq \sum_{n\geq 1}\frac{\kappa_n}{N^n}=\kappa^{(0)}+\lambda\kappa^{(1)}+O(\lambda^2)\,.$$

Note that (17) implies that

$$\frac{J_0(\lambda^{1/2}e^x)}{\lambda^{1/2}J_1(\lambda^{1/2})} = -x + \frac{\lambda}{4}(x+1+(x-1)e^{2x}) + O(\lambda^2),$$

so that

$$a_0 J_0(\lambda^{1/2} e^{\kappa/2 + \log|F_N(z)|}) = c_N \left( -\kappa/2 - \log|F_N(z)| + \frac{\lambda}{4} (\kappa/2 + \log|F_N(z)| + 1 + (\kappa/2 + \log|F_N(z)| - 1)e^{\kappa}|F_N(z)|^2) \right) + O(\lambda^2).$$

Similarly, we calculate the kernel K(z,t) to order  $O(\lambda^2)$  as

$$K(z,t) = 1 - \frac{\lambda}{4} e^{\kappa} F_N(\overline{z}) (F_N(z) - (t/z)^{1/N} F_N(t)) + O(\lambda^2).$$

If we first look at the boundary condition modulo  $O(\lambda)$ , it reads

$$\frac{1}{2}\kappa^{(0)} + \log|F_N(z)| = N^{-1} \operatorname{Re} \int_0^z V^{(0)}(t) \frac{dt}{t}, \qquad |z| = 1.$$

This clearly implies  $N^{-1} \int_0^z V^{(0)}(t) \frac{dt}{t} = \log F_N(z)$  and  $\kappa^{(0)} = 0$ . Using this we can rewrite the boundary condition for the linear term in  $\lambda$  as

$$\begin{split} &\frac{1}{2}\kappa^{(1)} - \frac{1}{4}(\log|F_N(z)| + 1 + (\log|F_N(z)| - 1)|F_N(z)|^2) - N^{-1}\operatorname{Re}\int\limits_0^z V^{(1)}(t)\frac{dt}{t} \\ &= -\frac{1}{4}N^{-1}\operatorname{Re}\int\limits_0^z V^{(0)}(t)F_N(\overline{z})(F_N(z) - (t/z)^{1/N}F_N(t))\frac{dt}{t} \,, \qquad |z| = 1 \,. \end{split}$$

Since  $N^{-1} \int_0^z V^{(0)}(t) \frac{dt}{t} = \log F_N(z)$ , we have  $V^{(0)}(t) = Nt \frac{F_N'(t)}{F_N(t)}$  and thus

$$\frac{1}{2}\kappa^{(1)} - \frac{1}{4}\log|F_N(z)| - N^{-1}\operatorname{Re}\int_0^z V^{(1)}(t)\frac{dt}{t} = \frac{1}{4}\Big(1 - |F_N(z)|^2 + \operatorname{Re}F_N(\overline{z})\widetilde{F}_N(z)\Big)$$

where we denote  $\widetilde{F}_N(z) = \int_0^z (t/z)^{1/N} F_N'(t) dt$ . Integrating over |z| = 1 leads to

$$2\kappa^{(1)} = \int_{0}^{1} \left( 1 - |F_N(e^{2\pi ix})|^2 + F_N(e^{-2\pi ix}) \widetilde{F}_N(e^{2\pi ix}) \right) dx.$$
 (23)

Our goal is to rewrite the right hand side of (23) as a hypergeometric series. For this we will make use of the integral representation for  $F_N(z)$ 

$$F_N(z) = 1 + \frac{1}{N} \int_0^1 t^{1/N} ((1 - tz)^{-2/N} - 1) \frac{dt}{t}.$$

First, we plug this representation into the definition of  $\widetilde{F}_N(z)$  to obtain

$$\widetilde{F}_N(z) = \frac{2}{N^2} \int_0^z (x/z)^{1/N} \left( \int_0^1 t^{1/N} (1 - xt)^{-2/N - 1} dt \right) dx$$

$$= \frac{2}{N^2} \int_0^1 \int_0^1 (t_1 t_2)^{1/N} z (1 - zt_1 t_2)^{-2/N - 1} dt_1 dt_2$$

$$= -\frac{2}{N^2} \int_0^1 t^{1/N} z (1 - zt)^{-2/N - 1} \log t dt.$$

From this, by changing the order of integration, we calculate

$$\int_{0}^{1} 1 - |F_{N}(e^{2\pi ix})|^{2} dx = -\frac{1}{N^{2}} \int_{0}^{1} \int_{0}^{1} (t_{1}t_{2})^{1/N-1} (G_{N}(t_{1}t_{2}) - 1) dt_{1} dt_{2},$$

$$\int_{0}^{1} F_{N}(e^{2\pi ix}) \widetilde{F}_{N}(e^{-2\pi ix}) dx = -\frac{1}{N^{2}} \int_{0}^{1} \int_{0}^{1} (t_{1}t_{2})^{1/N-1} t_{1} t_{2} G'_{N}(t_{1}t_{2}) \log t_{1} dt_{1} dt_{2},$$

where

$$G_N(x) = {}_2F_1(2/N, 2/N, 1; x) = \sum_{n \ge 0} \frac{(2/N)_n^2}{n!^2} x^n$$
.

Next, using the easily verified identity

$$\int_{0}^{1} \int_{0}^{1} f(xy) \log^{k} x \frac{dx}{x} \frac{dy}{y} = -\frac{1}{k+1} \int_{0}^{1} f(t) \log^{k+1} t \frac{dt}{t}$$

we can rewrite the above double integrals as single integrals. Plugging the resulting expressions back into (23) we get

$$2\kappa^{(1)} = \frac{1}{N^2} \int_0^1 ((G_N(t) - 1) \log t + \frac{t}{2} G_N'(t) \log^2 t) t^{1/N} \frac{dt}{t}.$$

Finally, expanding  $G_N(t)$  as a power series in t and integrating the above identity term-by-term we obtain

$$\kappa^{(1)} = -\frac{1}{2N^3} \sum_{n\geq 1} \frac{(2/N)_n^2}{n!^2 (1/N+n)^3},$$
(24)

which immediately implies (4).  $\square$ 

Finally, let us prove Theorem 3. For this we will need the following lemma to evaluate the right hand side of (24) in terms of gamma function and its derivatives.

**Lemma 4.** For all  $z \notin \frac{1}{2}\mathbb{Z}$  we have

$$\sum_{n=0}^{m} \frac{(2z)_n^2 z^3}{n!^2 (z+n)^3} \frac{(1+m)_n (-m)_n}{(1+2z+m)_n (2z-m)_n}$$

$$= \frac{(1+2z)_m (1-z)_m^2}{(1-2z)_m (1+z)_m^2} \left(1 + \sum_{j=1}^{m} \frac{j(j-2z)}{(j-z)^2} - \sum_{j=1}^{m} \frac{j(j+2z)}{(j+z)^2}\right)$$
(25)

**Proof.** We will prove this identity by induction on m, the case m = 0 being trivial. First, we divide both sides by the product of the Pochhammer symbols on the right to get an equivalent identity

$$\sum_{n=0}^{m} T_{n,m} = \frac{1}{z^3} \left( 1 + \sum_{j=1}^{m} \frac{j(j-2z)}{(j-z)^2} - \sum_{j=1}^{m} \frac{j(j+2z)}{(j+z)^2} \right),$$

where we denote

$$T_{n,m} := \frac{(1-2z)_m (1+z)_m^2}{(1+2z)_m (1-z)_m^2} \frac{(2z)_n^2}{n!^2 (z+n)^3} \frac{(1+m)_n (-m)_n}{(1+2z+m)_n (2z-m)_n}.$$

Then it is enough to show that

$$\sum_{m=0}^{m+1} (T_{n,m+1} - T_{n,m}) = -\frac{4(m+1)}{(m+1-z)^2(m+1+z)^2}.$$

First, an elementary calculation shows that for  $0 \le n \le m+1$  we have

$$T_{n,m+1} - T_{n,m} = \frac{4z(2z)_n^2}{n!^2(z+n)} \frac{(1-2z)_{m+1}(1+z)_m^2}{(1-z)_{m+1}^2(1+2z)_m} \frac{(1+m)_n(-m-1)_n}{(1+2z+m)_{n+1}(2z-m-1)_{n+1}}.$$

Therefore, it suffices to show that for  $m \geq 1$  we have

$$\sum_{n=0}^{m} D_{n,m} = 1,$$

where

$$D_{n,m} = -\frac{z(m-z)^2(2z)_n^2}{n!^2(z+n)m} \frac{(1-2z)_m(1+z)_m^2}{(1+2z)_{m+n}(1-z)_m^2} \frac{(m)_n(-m)_n}{(2z-m)_{n+1}}.$$

The last identity can be easily proved using the Wilf-Zeilberger method [26]. Explicitly, using the identities

$$\frac{D_{n,m+1}}{D_{n,m}} = \frac{(m+1+z)^2(m-n-2z)(m+n)(m+1)}{(m-z)^2(m+n+1+2z)m(m-n+1)}$$

$$\frac{D_{n+1,m}}{D_{n,m}} = \frac{(n+z)(n+2z)^2(m-n)(m+n)}{(n+1+z)(m-n-1-2z)(m+n+1+2z)(n+1)^2}$$

one can verify that

$$D_{n,m+1} - D_{n,m} = G_{n+1,m} - G_{n,m}, \qquad n = 0, \dots, m+1, \tag{26}$$

where  $G_{n,m} = D_{n,m}R(n,m)$  and

$$R(n,m) = \frac{n^2(2m+1)(z+n)(m-n-2z)(2m^2z+(m+z)^2-(n+z)^2+m+n+2z)}{4m^2(m+1)^2(n-m-1)(m-z)^2z} \,.$$

(We regularize  $G_{n,m}$  for n=m+1 by canceling the factor (n-m-1) in the denominator of R(n,m) with the factor (n-1-m) coming from the Pochhammer symbol  $(-m)_n$  in the definition of  $D_{n,m}$ .) Finally, the identity  $\sum_{n=0}^{m} D_{n,m} = 1$  then follows by induction on m from (26) together with  $G_{0,m} = G_{m+2,m} = 0$ .  $\square$ 

**Corollary 2.** For all  $z \in \mathbb{C}$  with |z| < 1 we have

$$\sum_{n\geq 0} \frac{(2z)_n^2 z^3}{n!^2 (z+n)^3} = \frac{\Gamma^2 (1+z) \Gamma (1-2z)}{\Gamma^2 (1-z) \Gamma (1+2z)} \left(1+z^2 \psi^{(1)} (1+z) - z^2 \psi^{(1)} (1-z)\right),\tag{27}$$

where  $\psi^{(k)}(z) = \frac{d^{k+1}}{dz^{k+1}} \log \Gamma(z)$  is the k-th polygamma function.

**Proof.** For Re z < 1 and  $z \notin \frac{1}{2}\mathbb{Z}$  simply take the limit  $m \to +\infty$  in (25) using the fact that  $(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)} \sim \frac{\Gamma(n)n^x}{\Gamma(x)}$ ,  $n \to \infty$ , together with

$$\sum_{j=1}^{m} \frac{j(j\pm 2z)}{(j\pm z)^2} = m - z^2 \psi^{(1)}(1\pm z) + z^2 \psi^{(1)}(1+m\pm z).$$

Noting that both sides of (27) are non-singular also for  $z=0,\pm 1/2$  we obtain the claim for all |z|<1.  $\square$ 

**Proof of Theorem 3.** The claim for  $C_n(0)$  immediately follows from (4) and (22). Differentiating the classical identity

$$\log \Gamma(1-z) = \gamma z + \sum_{n>2} \zeta(n) \frac{z^n}{n}$$

twice shows that

$$z^{2}\psi^{(1)}(1-z) - z^{2}\psi^{(1)}(1+z) = \sum_{k>1} 4k\zeta(2k+1)z^{2k+1},$$

and thus (4), (22) and (27) together imply the claim for  $C_n'(0)$ .  $\square$ 

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