
Volume 126, Number 6, June 2008 ISSN 0022-314X
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Journal of Number Theory 128 (2008) 1516–1554
JOURNAL OF Number Theory
www.elsevier.com/locate/jnt

Lower order terms in the full moment conjecture for the Riemann zeta function

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Received 30 December 2006

Available online 4 October 2007

Communicated by W. Luo

Abstract

We describe an algorithm for obtaining explicit expressions for lower terms for the conjectured full asymptotics of the moments of the Riemann zeta function, and give two distinct methods for obtaining numerical values of these coefficients. We also provide some numerical evidence in favor of the conjecture.

Keywords: L-functions; Random matrix theory; Moments

1. Introduction

In [CFKRS] the authors propose conjectures for the full asymptotics of the moments of L-functions. A sample conjecture states, for integer k, that the $2k$th moment of $|\zeta|$ on the half line can be estimated using a polynomial P_k of degree k^2, with the polynomial given implicitly as a $2k$-fold residue (see (1.2) below).

The leading term in the conjecture agrees with the Keating–Snaith conjecture [KS] for the leading asymptotics of the moments of ζ. Besides that, all the terms of the polynomial obtained

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0022-314X/$ – see front matter
doi:10.1016/j.jnt.2007.05.013

agrees with known theorems for $k = 1, 2$ [I,H-B], and the leading term agrees with conjectures made through earlier and distinct number theoretical methods for $k = 3, 4$ [CG,CGo].

The method used in [CFKRS] to conjecture the full asymptotics relies on number theoretic heuristics based on the approximate functional equation. The conjecture is supported by the fact that the formula coincides with an analogous expression in random matrix theory [CFKRS2] for the moments of characteristic polynomials from the unitary group, the main difference being that the moments of ζ have extra arithmetic information that does not show up for random matrices. Perhaps the most compelling support for the conjecture, though, are numerics that confirm the conjectured moments.

For those numerical confirmations it is necessary to use all terms arising in our heuristics. The purpose of this paper is to investigate the lower order degree terms which appear in the conjectured polynomials. Specifically, we

(1) describe an algorithm to obtain meromorphic expressions in k for the coefficients of the polynomial $P_k(x)$. Our main results are given in Theorems 1.2–1.4;
(2) explain how one can numerically compute the lower order terms and to provide further experimental confirmation of the full moment conjecture, including for non-integer values of k. Numerical values for the coefficients of these polynomials for $k = 1, 2, \ldots, 7$ are listed in [CFKRS] without explanation, with some numerics confirming the conjecture for $k = 3$.

At the end of the paper we also outline the analogous approach for moments of quadratic Dirichlet L-functions and of quadratic twists of an elliptic curve L-function, in both cases evaluated at the critical point. These two cases are examples of unitary-symplectic and orthogonal families respectively [KaS,KeS2,CF].

Before stating our results, we introduce notation and conjectures from [CFKRS].

1.1. Moment conjecture for ζ

Let

$$\Delta(z_1, \ldots, z_m) = \prod_{1 \leqslant i < j \leqslant m} (z_j - z_i) = \left|z_i^{j-1}\right|_{m \times m}$$

denote the Vandermonde determinant.

Conjecture. *(See [CFKRS].)*

For positive integer k, and any $\epsilon > 0$,

$$\int_0^T \left|\zeta(1/2 + it)\right|^{2k} dt = \int_0^T P_k\left(\log \frac{t}{2\pi}\right) dt + O\left(T^{1/2+\epsilon}\right), \tag{1.1}$$

with the constant in the O term depending on k and ϵ, where P_k is the polynomial of degree k^2 given implicitly by the $2k$-fold residue

$$P_k(x) = \frac{(-1)^k}{k!^2} \frac{1}{(2\pi i)^{2k}} \oint \cdots \oint \frac{G(z_1, \ldots, z_{2k}) \Delta^2(z_1, \ldots, z_{2k})}{\prod_{i=1}^{2k} z_i^{2k}} e^{\frac{x}{2} \sum_{i=1}^{k} z_i - z_{i+k}} \, dz_1 \ldots dz_{2k}, \tag{1.2}$$

with the path of integration over small circles about $z_i = 0$, where

$$G(z_1, \ldots, z_{2k}) = A_k(z_1, \ldots, z_{2k}) \prod_{i=1}^{k} \prod_{j=1}^{k} \zeta(1 + z_i - z_{j+k}), \tag{1.3}$$

and A_k is the Euler product

$$\begin{aligned} A_k(z_1, \ldots, z_{2k}) &\\ = \prod_p \prod_{i,j=1}^{k} \left(1 - p^{-1-z_i+z_{k+j}}\right) \int_0^1 \prod_{j=1}^{k} \left(1 - \frac{e(\theta)}{p^{\frac{1}{2}+z_j}}\right)^{-1} \left(1 - \frac{e(-\theta)}{p^{\frac{1}{2}-z_{k+j}}}\right)^{-1} d\theta & \quad (1.4) \\ = \prod_p \sum_{j=1}^{k} \prod_{i \neq j} \frac{\prod_{m=1}^{k} (1 - p^{-1+z_{i+k}-z_m})}{1 - p^{z_{i+k}-z_{j+k}}}. & \quad (1.5) \end{aligned}$$

Here $e(\theta) = \exp(2\pi i \theta)$.

We use both these expressions for the local factor for A_k. The first is used in obtaining meromorphic expressions in k for the coefficients of $P_k(x)$.

The second expression, derived in [CFKRS, 2.6], is used to numerically compute $A_k(z_1, \ldots, z_{2k})$ for specific values of $z_1, \ldots, z_{2k}$. The individual terms in the sum over j in (1.5) have poles (though these poles cancel out when summed over j, see the paragraph following [CFKRS, 2.6.16]) and when we numerically evaluate these terms individually, we take care to avoid the poles by making sure that the z_{j+k}'s are distinct.

The main point of the conjecture is that we believe it gives the full asymptotics of the moments of zeta. While our numerical results in Section 5 are consistent with a remainder of size $O(T^{1/2+\epsilon})$, there is some debate regarding the error, especially in relation to moments of other families of L-functions [CFKRS,Z], and it would be worthwhile to carry out more detailed testing concerning the nature of the remainder.

The leading coefficient of $P_k(x)$ will be shown in Section 2.1 to equal

$$a_k \prod_{j=0}^{k-1} \frac{j!}{(j+k)!}, \tag{1.6}$$

with

$$a_k = \prod_p \left(1 - p^{-1}\right)^{k^2} {}_2F_1(k, k; 1; 1/p) \tag{1.7}$$

and ${}_2F_1(a, b; c; t)$ the Gauss hypergeometric function

$$ {}_2F_1(a,b;c;t) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{t^n}{n!}. \tag{1.8} $$

This agrees with the leading term that was first conjectured by Keating and Snaith [KeS].

More generally, letting

$$ Z(s) = \chi(s)^{-1/2}\zeta(s) $$

with

$$ \chi(s) = \pi^{s-1/2}\Gamma\big((1-s)/2\big)/\,\Gamma(s/2) $$

we conjectured [CFKRS] for shifted moments

$$ \int_0^T Z(1/2+it+\alpha_1)\cdots Z(1/2+it+\alpha_{2k})\,dt \sim \int_0^T P_k\left(\alpha, \log\frac{t}{2\pi}\right)dt, \tag{1.9} $$

where

$$ P_k(\alpha,x) = \frac{(-1)^k}{k!^2}\frac{1}{(2\pi i)^{2k}} \oint\cdots\oint \frac{G(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_{2k})^2}{\prod_{i=1}^{2k}\prod_{j=1}^{2k}(z_i-\alpha_j)} e^{\frac{x}{2}\sum_{i=1}^{k} z_i - z_{i+k}}\,dz_1\dots dz_{2k}, \tag{1.10} $$

with the path of integration being small circles surrounding the poles α_i, and $-1/4 < \Re\alpha_j$. One recovers the moments of ζ by setting the shifts α_i equal to 0, and observing that $Z(s) = Z(1-s)$.

An alternative formulation of this conjecture also given in [CFKRS] involves a combinatorial sum and is established by the following lemma.

Lemma 1.1. *(See [CFKRS, Section 2.5].) Suppose $F(u;v) = F(u_1,\dots,u_k;v_1,\dots,v_k)$ is a function of $2k$ variables, symmetric with respect to the first k variables and also symmetric with respect to the second set of k variables. Suppose also that F is regular near $(0,\dots,0)$, and that $f(s)$ has a simple pole of residue 1 at $s=0$ but is otherwise analytic in a neighborhood about $s=0$. Let*

$$ H(u_1,\dots,u_k;v_1,\dots,v_k) = F(u_1,\dots;\dots,v_k)\prod_{i=1}^{k}\prod_{j=1}^{k} f(u_i-v_j). $$

If for all $1 \leqslant i,j \leqslant k$, $\alpha_i - \alpha_{j+k}$ is contained in the region of analyticity of $f(s)$ then

$$ \frac{(-1)^k}{k!^2}\frac{1}{(2\pi i)^{2k}} \oint\cdots\oint \frac{H(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_{2k})^2}{\prod_{i=1}^{2k}\prod_{j=1}^{2k}(z_i-\alpha_j)}\,dz_1\dots dz_{2k} = \sum_{\sigma\in\Xi} H(\alpha_{\sigma(1)},\dots,\alpha_{\sigma(2k)}), \tag{1.11} $$

where one integrates about small circles enclosing the α_j's, and where Ξ is the set of $\binom{2k}{k}$ permutations $\sigma \in S_{2k}$ such that $\sigma(1) < \cdots < \sigma(k)$ and $\sigma(k+1) < \cdots < \sigma(2k)$.

Equation (1.2) allows us to obtain the coefficients of $P_k(x)$ by computing power series expansions and then the residue of the r.h.s., giving meromorphic expressions in k for the coefficients which can also be evaluated to high precision numerically, even for non integer k. In practice we have been able to do so for the first ten coefficients of $P_k(x)$. If $k \in \mathbb{Z}$, $k > 3$, to obtain numerical values for all k^2 coefficients of $P_k(x)$ we developed a second method using Eq. (1.11). This involved taking small distinct shifts and high working precision to capture cancellation amongst the order k^2 poles of the r.h.s. of (1.11).

1.2. Results

Our first theorem below explicitly gives the coefficients of $P_k(x)$ in the full moment conjecture for the Riemann zeta function. These are described in terms of the multivariate Taylor coefficients of

$$\frac{1}{a_k} A_k(z_1, \ldots, z_{2k}) \prod_{1 \leqslant i,j \leqslant k} (z_i - z_{j+k}) \zeta(1 + z_i - z_{j+k}). \tag{1.12}$$

We let $b_k(\alpha; \beta)$ denote the coefficient of $z_1^{\alpha_1} \cdots z_k^{\alpha_k} z_{k+1}^{\beta_1} \cdots z_{2k}^{\beta_k}$ in the Taylor series of (1.12). Let

$$|\alpha| = \sum_1^k \alpha_i \tag{1.13}$$

and likewise for β. Notice that the function in (1.12) is symmetric in $z_1, \ldots, z_k$ and in $z_{k+1}, \ldots, z_{2k}$, and that $b_k(\alpha; \beta) = (-1)^{|\alpha|+|\beta|} b_k(\beta; \alpha)$. We may therefore collect together terms in the Taylor series accordingly and express (1.12) as

$$\sum_{\alpha;\beta} b_k(\alpha; \beta) \big(z_1^{\alpha_1} \cdots z_k^{\alpha_k} z_{k+1}^{\beta_1} \cdots z_{2k}^{\beta_k} \pm \text{sym} \big). \tag{1.14}$$

The 'sym' indicates that we group terms that have exponents of the same form. Thus the sum over $\alpha; \beta$ follows the convention that $\alpha \geqslant \beta$ lexicographically, we list the α_i's and β_i's in decreasing order, and we suppress the α_i's and β_i's that are 0. For example, all the terms of degree 4 are collected with coefficients: $b_k(1,1,1,1;)$, $b_k(2,1,1;)$, $b_k(2,2;)$, $b_k(3,1;)$, $b_k(4;)$, $b_k(1,1,1;1)$, $b_k(2,1;1)$, $b_k(3;1)$, $b_k(1,1;1,1)$, $b_k(2;1,1)$, $b_k(2;2)$. The terms that go with $b_k(1,1,1,1;)$ are

$$\sum_{1 \leqslant i_1 < i_2 < i_3 < i_4 \leqslant k} z_{i_1} z_{i_2} z_{i_3} z_{i_4} + z_{k+i_1} z_{k+i_2} z_{k+i_3} z_{k+i_4}.$$

Theorem 1.2. *Let $P_k(x)$ be given by Eq.* (1.2)*. Writing*

$$P_k(x) = c_0(k) x^{k^2} + c_1(k) x^{k^2-1} + \cdots + c_{k^2}(k), \tag{1.15}$$

we have

$$c_r(k) = a_k \prod_{l=0}^{k-1} \frac{l!}{(k+l)!} \sum_{|\alpha|+|\beta|=r} 2^{1-\delta(\alpha;\beta)} b_k(\alpha;\beta) N_k(\alpha;\beta), \tag{1.16}$$

where a_k is given by (1.7)*, the function $\delta(\alpha;\beta)$ equals zero unless $\alpha = \beta$ in which case it equals* 1*, and $N_k(\alpha;\beta)$ is defined by*

$$N_k(\alpha;\beta) = \frac{1}{2^{k^2-r}} \left(\prod_{l=0}^{k-1} \frac{l!}{(k+l)!} \right)^{-1} \sum_{\substack{\text{rearrangements} \\ \sigma,\tau \text{ of } \alpha \text{ and } \beta}} \tilde{M}_k\big(\sigma(\alpha), \tau(\beta)\big). \tag{1.17}$$

The function $\tilde{M}_k$ is given as a $2k \times 2k$ determinant in Eq. (2.63).

By rearrangements, we mean distinct permutations. Two permuatations $\sigma(\alpha)$ and $\mu(\alpha)$ are said to be distinct if $\alpha_{\sigma_i} \neq \alpha_{\mu_i}$ for some i. For example, if $\alpha_1 = 7$, $\alpha_2 = 5$, $\alpha_3 = 5$ then the two permutations $\alpha_2, \alpha_1, \alpha_3$ and $\alpha_3, \alpha_1, \alpha_2$ are not distinct and would only be counted once in (1.17).

The reason for writing $N_k(\alpha;\beta)$ as we have, with the factor $(\prod_{l=0}^{k-1} \frac{l!}{(k+l)!})^{-1}$, is explained by the next theorem.

Theorem 1.3. *$N_k(\alpha;\beta)$ is a polynomial in k of degree $\leqslant 2(|\alpha| + |\beta|)$.*

This theorem allows us to determine $N_k(\alpha;\beta)$ explicitly by evaluating (1.17) at $2(|\alpha| + |\beta|) + 1$ values of k and interpolating. A few example $N_k(\alpha;\beta)$'s are given in (2.70).

Finally, the coefficients $b_k(\alpha;\beta)$ that appear in Theorem 1.2 can also be explicitly determined.

Theorem 1.4. *The Taylor coefficients $b_k(\alpha;\beta)$ of* (1.12) *can be written explicitly as a polynomial in: k, the Taylor coefficients of $s\zeta(1+s)$, and the Taylor coefficients of* $\log(A_k(z_1,\dots,z_{2k}))$*. The latter Taylor coefficients can further be expressed explicitly as a sum over all primes p of a rational function in: k, p,* $\log(p)$*, and finitely many Gauss hypergeometric functions ${}_2F_1(k_1,k_2;m;1/p)$, where $k_1, k_2, m \in \mathbb{Z}$, $k_1, k_2 \geqslant k$ and $m \geqslant 1$.*

To illustrate what the last theorem looks like in practice, see Eqs. (2.51) and (2.43).

This paper is structured as follows. In Section 2.1 we prove Theorems 1.2 and 1.4, and also give a procedure to determine the polynomial and rational functions of Theorem 1.4. In Section 3 we prove Theorem 1.3.

Section 4 is devoted to numerical evaluation of the lower order terms. Two different methods are described. The first involves numerically computing the terms that appear in Theorem 1.2, while the second uses (1.11), small shifts, and very high precision to capture cancellation amongst the poles of the summand. Data supporting the full moment conjecture is then presented in Section 5.

We also provide plots of the coefficients $c_r(k)$ as a function of k for $r \leqslant 7$ and also of the zeros of the polynomials $P_k(x)$ for several values of k.

In Section 6 we briefly describe the analogous approach for quadratic Dirichlet L-functions and of quadratic twists of an elliptic curve L-function.

2. Lower order terms in the moments of ζ

2.1. Evaluating the residue explicitly

The $2k$-fold residue in (1.2) involves extracting the coefficient of $\prod_1^{2k} z_i^{2k-1}$, i.e. a polynomial of degree $2k(2k-1)$. The Vandermonde determinant has degree $2\binom{2k}{2} = 2k(2k-1)$. However, the product $\prod_{i=1}^{k}\prod_{j=1}^{k}\zeta(1+z_i-z_{j+k})$ has poles which cancel k^2 of the Vandermonde factors. Hence, in (1.2), we need only take terms in the Taylor expansion of $\exp(\frac{x}{2}\sum_{i=1}^{k} z_i - z_{i+k})$ up to degree k^2. Therefore, $P_k(x)$ is indeed a polynomial of degree k^2 in x and we write

$$P_k(x) = c_0(k)x^{k^2} + c_1(k)x^{k^2-1} + c_2(k)x^{k^2-2} + \cdots + c_{k^2}(k). \tag{2.1}$$

One complication in developing expressions in k for the $c_r(k)$'s is that the Vandermonde determinant in (1.2) prevents us from separating the integrals. However, this can be overcome by introducing extra variables and pulling out the Vandermonde as a differential operator. We illustrate the method for the leading term $c_0(k)$ and then generalize.

Noticing that $A_k(0,0,\dots,0) = a_k$ (set all the variables to 0 in (1.4), apply Lemma 2.3, and compare to (1.7)), the leading term is given by

$$c_0(k)x^{k^2} = \frac{a_k}{k!^2}\frac{1}{(2\pi i)^{2k}}\oint\cdots\oint \Delta(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_k)\Delta(z_{k+1},\dots,z_{2k}) \times \frac{\exp(\frac{x}{2}\sum_{i=1}^{k} z_i - z_{i+k})}{\prod_{i=1}^{2k} z_i^{2k}}\, dz_1\dots dz_{2k} \tag{2.2}$$

(the k^2 poles of the ζ product have sign opposite from the Vandermonde factors that they cancel, and these k^2 minuses cancel the $(-1)^k$ in (1.2)). Comparing the degree of the Vandermonde determinants in the numerator, with the degree of the denominator shows that only terms of degree k^2 in the Taylor expansion of the exp contribute to the residue. Changing variables $u_i = xz_i/2$ and then relabeling u_i with z_i gives

$$\frac{x^{k^2}}{2^{k^2}}\frac{a_k}{k!^2}\frac{1}{(2\pi i)^{2k}}\oint\cdots\oint \Delta(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_k)\Delta(z_{k+1},\dots,z_{2k}) \times \frac{\exp(\sum_{i=1}^{k} z_i - z_{i+k})}{\prod_{i=1}^{2k} z_i^{2k}}\, dz_1\dots dz_{2k}. \tag{2.3}$$

Introducing extra variables x_i, we consider

$$\frac{1}{(2\pi i)^{2k}}\oint\cdots\oint p(z_1,\dots,z_{2k})\frac{\exp(\sum_{i=1}^{2k} x_i z_i)}{\prod_{i=1}^{2k} z_i^{2k}}\, dz_1\dots dz_{2k} \tag{2.4}$$

with $p(z)$ a polynomial in $z_1,\dots,z_{2k}$. Pulling out the polynomial p, (2.4) equals

$$p(\partial/\partial x_1,\dots,\partial/\partial x_{2k})\frac{1}{(2\pi i)^{2k}}\oint\cdots\oint \frac{\exp(\sum_{i=1}^{2k} x_i z_i)}{\prod_{i=1}^{2k} z_i^{2k}}\, dz_1\dots dz_{2k}, \tag{2.5}$$

and taking the residue gives

$$p(\partial/\partial x_1,\ldots,\partial/\partial x_{2k})\prod_1^{2k}\frac{x_i^{2k-1}}{(2k-1)!}. \tag{2.6}$$

Therefore, (2.3) equals

$$\frac{x^{k^2}}{2^{k^2}}\frac{a_k}{k!^2}q(\partial/\partial x_1,\ldots,\partial/\partial x_{2k})\prod_1^{2k}\frac{x_i^{2k-1}}{(2k-1)!} \tag{2.7}$$

evaluated at $x_1=\cdots=x_k=1$, $x_{k+1}=\cdots=x_{2k}=-1$, with

$$q(\partial/\partial x_1,\ldots,\partial/\partial x_{2k})=\Delta(\partial/\partial x_1,\ldots,\partial/\partial x_{2k})\Delta(\partial/\partial x_1,\ldots,\partial/\partial x_k)\Delta(\partial/\partial x_{k+1},\ldots,\partial/\partial x_{2k}). \tag{2.8}$$

Two lemmas allow us to reduce this further.

Lemma 2.1.

$$\Delta(\partial/\partial x_1,\ldots,\partial/\partial x_n)\prod_1^{n}f(x_i)=\left|f^{(j-1)}(x_i)\right|_{n\times n}.$$

Proof. This follows using the definition of the Vandermonde determinant

$$\Delta(\partial/\partial x_1,\ldots,\partial/\partial x_n)=\left|\partial^{j-1}/\partial x_i^{j-1}\right|_{n\times n}.$$

Noticing that row i of the matrix only involves x_i, we factor the product into the determinant. □

We can now consider the effect of applying the three Vandermonde's in (2.8).

Lemma 2.2.

$$\Delta(\partial/\partial x_1,\ldots,\partial/\partial x_{2k})\Delta(\partial/\partial x_1,\ldots,\partial/\partial x_k)\Delta(\partial/\partial x_{k+1},\ldots,\partial/\partial x_{2k})\prod_1^{2k}f(x_i)$$

evaluated at $x_1=\cdots=x_k=1$, $x_{k+1}=\cdots=x_{2k}=-1$ *equals*

$$k!^2\begin{vmatrix} f(1) & f^{(1)}(1) & \ldots & f^{(2k-1)}(1)\\ f^{(1)}(1) & f^{(2)}(1) & \ldots & f^{(2k)}(1)\\ \vdots & \vdots & \ddots & \vdots\\ f^{(k-1)}(1) & f^{(k)}(1) & \ldots & f^{(3k-2)}(1)\\ f(-1) & f^{(1)}(-1) & \ldots & f^{(2k-1)}(-1)\\ f^{(1)}(-1) & f^{(2)}(-1) & \ldots & f^{(2k)}(-1)\\ \vdots & \vdots & \ddots & \vdots\\ f^{(k-1)}(-1) & f^{(k)}(-1) & \ldots & f^{c(3k-2)}(-1)\end{vmatrix}_{2k\times 2k}$$

(*the first k rows of this $2k \times 2k$ matrix involve f and its derivatives evaluated at* 1*, while the last k rows have the entries evaluated at* -1).

Proof. Consider first what happens when we apply just the last two Δ's. By Lemma 2.1,

$$\Delta(\partial/\partial x_1, \dots, \partial/\partial x_k)\Delta(\partial/\partial x_{k+1}, \dots, \partial/\partial x_{2k}) \prod_1^{2k} f(x_i) = \begin{vmatrix} A_{k\times k} & 0_{k\times k} \\ 0_{k\times k} & B_{k\times k} \end{vmatrix} \tag{2.9}$$

with

$$A_{i,j} = f^{(j-1)}(x_i), \tag{2.10}$$

$$B_{i,j} = f^{(j-1)}(x_{i+k}). \tag{2.11}$$

Expanding this determinant, we get a sum of $(k!)^2$ terms each of which is a product of the form

$$\operatorname{sgn}(\mu)\operatorname{sgn}(\nu) \prod_{i=1}^{k} f^{(\mu_i-1)}(x_i) f^{(\nu_i-1)}(x_{i+k}) \tag{2.12}$$

where $\mu_1, \dots, \mu_k$ and $\nu_1, \dots, \nu_k$ are permutations of the numbers $1, 2, \dots, k$. Applying the third Vandermonde $\Delta(\partial/\partial x_1, \dots, \partial/\partial x_{2k})$ to a typical such term gives, by Lemma 2.1,

$$\operatorname{sgn}(\mu)\operatorname{sgn}(\nu) \begin{vmatrix} f^{(\mu_1-1)}(x_1) & f^{(\mu_1)}(x_1) & \dots & f^{(\mu_1+2k-2)}(x_1) \\ f^{(\mu_2-1)}(x_2) & f^{(\mu_2)}(x_2) & \dots & f^{(\mu_2+2k-2)}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f^{(\mu_k-1)}(x_k) & f^{(\mu_k)}(x_k) & \dots & f^{(\mu_k+2k-2)}(x_k) \\ f^{(\nu_1-1)}(x_{k+1}) & f^{(\nu_1)}(x_{k+1}) & \dots & f^{(\nu_1+2k-2)}(x_{k+1}) \\ f^{(\nu_2-1)}(x_{k+2}) & f^{(\nu_2)}(x_{k+2}) & \dots & f^{(\nu_2+2k-2)}(x_{k+2}) \\ \vdots & \vdots & \ddots & \vdots \\ f^{(\nu_k-1)}(x_{2k}) & f^{(\nu_k)}(x_{2k}) & \dots & f^{(\nu_k+2k-2)}(x_{2k}) \end{vmatrix}_{2k\times 2k}. \tag{2.13}$$

Setting $x_1 = \dots = x_k = 1$, $x_{k+1} = \dots = x_{2k} = -1$, we may rearrange the first k rows and the last k rows so as to undo the permutations μ and ν. This introduces another $\operatorname{sgn}(\mu)\operatorname{sgn}(\nu)$ in front of the determinant. Hence each such term contributes the same amount,

$$\begin{vmatrix} f(1) & f^{(1)}(1) & \dots & f^{(2k-1)}(1) \\ f^{(1)}(1) & f^{(2)}(1) & \dots & f^{(2k)}(1) \\ \vdots & \vdots & \ddots & \vdots \\ f^{(k-1)}(1) & f^{(k)}(1) & \dots & f^{(3k-2)}(1) \\ f(-1) & f^{(1)}(-1) & \dots & f^{(2k-1)}(-1) \\ f^{(1)}(-1) & f^{(2)}(-1) & \dots & f^{(2k)}(-1) \\ \vdots & \vdots & \ddots & \vdots \\ f^{(k-1)}(-1) & f^{(k)}(-1) & \dots & f^{(3k-2)}(-1) \end{vmatrix}_{2k\times 2k}, \tag{2.14}$$

and summing over the $(k!)^2$ pairs μ, ν gives us the lemma. □

Applying Lemma 2.2 to (2.7) yields

$$c_0(k) = \frac{a_k}{2^{k^2}} \begin{vmatrix} \Gamma(2k)^{-1} & \Gamma(2k-1)^{-1} & \dots & \Gamma(1)^{-1} \\ \Gamma(2k-1)^{-1} & \Gamma(2k-2)^{-1} & \dots & \Gamma(0)^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma(k+1)^{-1} & \Gamma(k)^{-1} & \dots & \Gamma(-k+2)^{-1} \\ -\Gamma(2k)^{-1} & \Gamma(2k-1)^{-1} & \dots & \Gamma(1)^{-1} \\ \Gamma(2k-1)^{-1} & -\Gamma(2k-2)^{-1} & \dots & -\Gamma(0)^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^k\Gamma(k+1)^{-1} & (-1)^{k+1}\Gamma(k)^{-1} & \dots & (-1)^{3k-1}\Gamma(-k+2)^{-1} \end{vmatrix}_{2k\times 2k} . \tag{2.15}$$

Here, we take $\Gamma(m)^{-1} = 0$ if $m \in \{0, -1, -2, -3, \ldots\}$. The first k rows and last k rows are identical except for the presence of a checkerboard pattern of minus ones in the latter rows. The i, j entry above equals

$$\begin{cases} \Gamma(2k-i-j+2)^{-1}, & \text{if } 1 \leqslant i \leqslant k; \\ (-1)^{i+j-k-1}\Gamma(3k-i-j+2)^{-1} & \text{if } k+1 \leqslant i \leqslant 2k. \end{cases} \tag{2.16}$$

We show later that (2.15) equals $a_k \prod_{l=0}^{k-1} l!/(k+l)!$. See Lemma 3.1 and Theorem 3.2, with $e_i = f_i = 0$, $c_i = k+i-1$.

Next we consider in (2.1) the rth term of our polynomial $P_k(x)$. To evaluate $c_r(k)$ we examine the power series expansion of the integrand in (1.2). As in our consideration of $c_0(k)$, we first cancel the poles of $\prod_{i=1}^{k}\prod_{j=1}^{k}\zeta(1+z_i-z_{j+k})$ against the Vandermonde, and write the integral in (1.2) as

$$\begin{aligned} P_k(x) = \frac{1}{k!^2}\frac{1}{(2\pi i)^{2k}} \oint \cdots \oint & \frac{\Delta(z_1,\ldots,z_{2k})\Delta(z_1,\ldots,z_k)\Delta(z_{k+1},\ldots,z_{2k})}{\prod_{i=1}^{2k} z_i^{2k}} \\ & \times A_k(z_1,\ldots,z_{2k}) \prod_{1\leqslant i,j\leqslant k}(z_i - z_{j+k})\zeta(1+z_i-z_{j+k}) \\ & \times e^{\frac{x}{2}\sum_{i=1}^{k} z_i - z_{i+k}}\, dz_1 \ldots dz_{2k}. \end{aligned} \tag{2.17}$$

Because of the various symmetries satisfied by the factors of the integrand, our job of determining the series expansion of

$$A_k(z_1,\ldots,z_{2k}) \prod_{1\leqslant i,j\leqslant k}(z_i - z_{j+k})\zeta(1+z_i-z_{j+k}) \tag{2.18}$$

is not as difficult as might be supposed.

2.1.1. Series for $A_k(z_1,\dots,z_{2k})$

First, we write

$$A_k(z_1,\dots,z_{2k}) = \exp\bigl(\log\bigl(A_k(z_1,\dots,z_{2k})\bigr)\bigr) \tag{2.19}$$

to turn the Euler product defining A_k in (1.5) into a sum over primes. Obtaining the series for $\log(A_k(z_1,\dots,z_{2k}))$ will allow us, in conjunction with the method in Section 2.1.3 for multiplying series, to recover the series for $\exp(\log(A_k(z_1,\dots,z_{2k})))$.

Because $A_k(z_1,\dots,z_{2k})$ is symmetric in $z_1,\dots,z_k$ and separately in $z_{k+1},\dots,z_{2k}$, we distinguish two sets of variables, and let

$$B_k(\alpha_1,\alpha_2,\dots,\alpha_k;\beta_1,\beta_2,\dots,\beta_k) \tag{2.20}$$

denote the coefficient of a typical

$$\frac{z_1^{\alpha_1}}{\alpha_1!}\cdots\frac{z_k^{\alpha_k}}{\alpha_k!}\frac{z_{k+1}^{\beta_1}}{\beta_1!}\cdots\frac{z_{2k}^{\beta_k}}{\beta_k!} \tag{2.21}$$

in the multivariate Taylor expansion of $\log(A_k(z_1,\dots,z_{2k}))$. Here, we prefer to keep factorials in the denominator rather than absorb them into B_k for convenience in describing the procedure to obtain the coefficients through differentiation.

By the above mentioned symmetry, we use the convention, when writing $B_k(\alpha;\beta)$ of only listing the non-zero α_i's and β_i's, and writing them in decreasing order. Also, because

$$A_k(z_1,\dots,z_{2k}) = A_k(-z_{k+1},\dots,-z_{2k},-z_1,\dots,-z_{k+1}) \tag{2.22}$$

we have

$$B_k(\alpha;\beta) = (-1)^{|\alpha|+|\beta|}B_k(\beta;\alpha) \tag{2.23}$$

where $|\alpha| = \sum_1^k \alpha_i$. Therefore

$$\begin{aligned} A_k(z_1,\dots,z_{2k}) = a_k\exp\Biggl(& B_k(1;)\sum_1^k z_i - z_{i+k} + B_k(1,1;)\sum_{1\leqslant i<j\leqslant k} z_iz_j + z_{i+k}z_{j+k} \\ &+ B_k(1;1)\sum_{1\leqslant i,j\leqslant k} z_iz_{j+k} + B_k(2;)\sum_1^{2k}\frac{z_i^2}{2} \\ &+ B_k(1,1,1;)\sum_{1\leqslant i<j<l\leqslant k} z_iz_jz_l - z_{i+k}z_{j+k}z_{l+k} + \cdots\Biggr). \end{aligned} \tag{2.24}$$

The a_k factor comes from the value of the function at the origin $A_k(0,\dots,0) = a_k$.

Next, let $l = l(\alpha)$ denote the number of non-zero α_i's, and $m = m(\beta)$ denote the number of non-zero β_i's. Since we are interested in extracting $c_r(k)$, we only need to consider the power series expansion of A_k up to degree r, i.e. $l + m \leqslant r$. Since we are assuming in our evaluation of $B_k(\alpha;\beta)$ that the α_i's and β_i's are in decreasing order, we focus on the first l z_i's (m z_{i+k}'s respectively) and we have, together with (1.5),

$$B_k(\alpha;\beta) = \sum_p \prod_{i=1}^{l} \frac{\partial^{\alpha_i}}{\partial z_i^{\alpha_i}} \prod_{i=1}^{m} \frac{\partial^{\beta_i}}{\partial z_{i+k}^{\beta_i}} \log\bigl(f_k(1/p;z)\bigr)\Big|_{z=0} \tag{2.25}$$

where

$$f_k(t;z) = \prod_{1\leqslant i,j\leqslant k} \bigl(1 - t^{1+z_i-z_{k+j}}\bigr) \int_0^1 \prod_{j=1}^{k} \bigl(1 - e(\theta)t^{\frac{1}{2}+z_j}\bigr)^{-1} \bigl(1 - e(-\theta)t^{\frac{1}{2}-z_{k+j}}\bigr)^{-1}\, d\theta. \tag{2.26}$$

Since we are assuming $\alpha_{l+1} = \cdots = \alpha_k = 0$, $\beta_{m+1} = \cdots = \beta_k = 0$, with $l + m \leqslant r$, we may as well immediately set $z_{r+1} = \cdots = z_k = 0$, $z_{k+r+1} = \cdots = z_{2k} = 0$. Therefore,

$$\sum_{1\leqslant i,j\leqslant k} \log\bigl(1 - t^{1+z_i-z_{k+j}}\bigr) \equiv \sum_{1\leqslant i,j\leqslant r} \log\bigl(1 - t^{1+z_i-z_{k+j}}\bigr) + \sum_{i=1}^{r} (k-r)\bigl(\log\bigl(1 - t^{1+z_i}\bigr) + \log\bigl(1 - t^{1-z_{i+k}}\bigr)\bigr). \tag{2.27}$$

By equivalent, we mean that both expressions have the same series expansion in z up to terms involving just $z_1, \ldots, z_r$, though not including the constant which, on the l.h.s., equals $k^2 \log(1-t)$. The main point in doing this reduction is to get rid of the k dependence in the summands.

A symbolic differentiation package (such as Maple) can then be used to compute

$$\prod_{i=1}^{l} \frac{\partial^{\alpha_i}}{\partial z_i^{\alpha_i}} \prod_{i=1}^{m} \frac{\partial^{\beta_i}}{\partial z_{i+k}^{\beta_i}} \Big|_{z=0} \tag{2.28}$$

applied to the r.h.s. of (2.27) as a rational function in k, $\log(t)$, and t. We list the terms up to degree 2:

$$\sum_{1\leqslant i,j\leqslant k} \log\bigl(1 - t^{1+z_i-z_{k+j}}\bigr) = k^2 \log(1-t) - \frac{kt\log(t)}{1-t} \sum_1^k z_i - z_{i+k} + \frac{t\log(t)^2}{(1-t)^2} \sum_{1\leqslant i,j\leqslant k} z_i z_{j+k} - \frac{kt\log(t)^2}{(1-t)^2} \sum_1^{2k} \frac{z_i^2}{2} + \cdots. \tag{2.29}$$

The coefficient above of the $\sum_{1\leqslant i<j\leqslant k} z_i z_j + z_{i+k} z_{j+k}$ term equals zero.

Next, applying (2.28) to

$$\log\left(\int_0^1 \prod_{j=1}^{k} \bigl(1 - e(\theta)t^{\frac{1}{2}+z_j}\bigr)^{-1} \bigl(1 - e(-\theta)t^{\frac{1}{2}-z_{k+j}}\bigr)^{-1}\, d\theta\right) \tag{2.30}$$

we end up, by the chain rule, with a rational expression involving partial derivatives of the form

$$\prod_{i=1} \frac{\partial^{c_i}}{\partial z_i^{c_i}} \prod_{i=1} \frac{\partial^{d_i}}{\partial z_{i+k}^{d_i}} \int_0^1 \prod_{j=1}^{k} \bigl(1 - e(\theta) t^{\frac{1}{2}+z_j}\bigr)^{-1} \bigl(1 - e(-\theta) t^{\frac{1}{2}-z_{k+j}}\bigr)^{-1} \, d\theta \Big|_{z=0}. \tag{2.31}$$

Now,

$$\bigl(1 - e(\theta) t^{\frac{1}{2}+z}\bigr)^{-1} = \sum_{m=0}^{\infty} \bigl(e(\theta) t^{\frac{1}{2}+z}\bigr)^m \tag{2.32}$$

so

$$\frac{\partial^c}{\partial z^c} \bigl(1 - e(\theta) t^{\frac{1}{2}+z}\bigr)^{-1} \Big|_{z=0} = \log(t)^c \sum_{m=0}^{\infty} \bigl(e(\theta) t^{\frac{1}{2}}\bigr)^m m^c. \tag{2.33}$$

The sum above is of the form

$$\sum_{m=0}^{\infty} w^m m^c \tag{2.34}$$

which can be evaluate by applying $(wd/dw)^c$ to the geometric series $1/(1-w) = \sum_{m=0}^{\infty} w^m$. This can be expressed either in terms of Stirling numbers of the second kind or, alternatively in terms of Eulerian numbers [St]:

$$\sum_{m=0}^{\infty} w^m m^c = \sum_{l=0}^{c} l! S(l,i) w^l (1-w)^{-l-1} = (1-w)^{-c-1} \sum_{l=0}^{c-1} E(c,l) w^{l+1} \tag{2.35}$$

(the latter sum is taken to be 1 if $c = 0$). We prefer to use the latter. Thus, (2.33) equals

$$\log(t)^c \bigl(1 - e(\theta) t^{\frac{1}{2}}\bigr)^{-c-1} \sum_{l=0}^{c-1} E(c,l) e\bigl((l+1)\theta\bigr) t^{(l+1)/2}. \tag{2.36}$$

Likewise,

$$\frac{\partial^d}{\partial z^d} \bigl(1 - e(-\theta) t^{\frac{1}{2}-z}\bigr)^{-1} \Big|_{z=0} = \bigl(-\log(t)\bigr)^d \bigl(1 - e(-\theta) t^{\frac{1}{2}}\bigr)^{-d-1} \sum_{l=0}^{d-1} E(d,l) e\bigl(-(l+1)\theta\bigr) t^{(l+1)/2}. \tag{2.37}$$

Applying this to (2.31) and expanding out, we need to evaluate integrals of the form

$$\int_0^1 \bigl(1 - e(\theta) t^{1/2}\bigr)^{-k-\sum c_i} \bigl(1 - e(-\theta) t^{1/2}\bigr)^{-k-\sum d_i} e(C\theta) \, d\theta \tag{2.38}$$

where $C \in \mathbb{Z}$, $-\sum d_i \leqslant C \leqslant \sum c_i$. The integral above can be expressed in terms of Gauss' hypergeometric series.

Lemma 2.3. *Let $A, B, C \in \mathbb{Z}$, $A, B \geqslant 1$, $0 \leqslant t < 1$. If $C \geqslant 0$ then*

$$\int_0^1 \left(1 - e(\theta)t^{1/2}\right)^{-A}\left(1 - e(-\theta)t^{1/2}\right)^{-B} e(C\theta)\, d\theta = t^{C/2}\binom{B+C-1}{C}\,{}_2F_1(A, B+C; C+1; t). \tag{2.39}$$

If $C < 0$, then

$$\int_0^1 \left(1 - e(\theta)t^{1/2}\right)^{-A}\left(1 - e(-\theta)t^{1/2}\right)^{-B} e(C\theta)\, d\theta = t^{|C|/2}\binom{A+|C|-1}{|C|}\,{}_2F_1(B, A+|C|; |C|+1; t). \tag{2.40}$$

Proof. Assume $C \geqslant 0$. We can expand $(1 - e(\theta)t^{1/2})^{-A}$ and $(1 - e(-\theta)t^{1/2})^{-B}$ using the binomial series:

$$\begin{aligned}
\left(1 - e(\theta)t^{1/2}\right)^{-A} &= 1 + Ae(\theta)t^{1/2} + \frac{A(A+1)}{2!}\left(e(\theta)t^{1/2}\right)^2 \\
&\quad + \frac{A(A+1)(A+2)}{3!}\left(e(\theta)t^{1/2}\right)^3 + \cdots, \\
\left(1 - e(-\theta)t^{1/2}\right)^{-B} &= 1 + Be(-\theta)t^{1/2} + \frac{B(B+1)}{2!}\left(e(-\theta)t^{1/2}\right)^2 \\
&\quad + \frac{B(B+1)(B+2)}{3!}\left(e(-\theta)t^{1/2}\right)^3 + \cdots.
\end{aligned}$$

Multiply these series together. The integral will pull out the coefficient of $e(-C\theta)$, which equals

$$\begin{aligned}
&t^{C/2}\left(\frac{B\ldots(B+C-1)}{C!} + \frac{B\ldots(B+C)}{(C+1)!}At + \frac{B\ldots(B+C+1)}{(C+2)!}\frac{A(A+1)}{2!}t^2 + \cdots\right) \\
&\quad = t^{C/2}\binom{B+C-1}{C}\,{}_2F_1(A, B+C; C+1; t).
\end{aligned} \tag{2.41}$$

The second formula in the lemma can be obtained by conjugating the first and interchanging the role of A and B. $\square$

Using this lemma, we can write out the Taylor series of (2.30)

$$\log\left(\int_0^1 \prod_{j=1}^k \left(1-e(\theta)t^{\frac{1}{2}+z_j}\right)^{-1}\left(1-e(-\theta)t^{\frac{1}{2}-z_{k+j}}\right)^{-1}d\theta\right)$$

$$\begin{aligned}
&= \log\left({}_2F_1(k,k;1;t)\right) + \frac{t\log(t)k\,{}_2F_1(k+1,k+1;2;t)}{{}_2F_1(k,k;1;t)}\sum_1^k z_i - z_{i+k}\\
&\quad + \left(\frac{-(t\log(t))^2k^2\,{}_2F_1(k+1,k+1;2;t)^2}{{}_2F_1(k,k;1;t)^2} + \frac{(t\log(t))^2\binom{k+1}{2}\,{}_2F_1(k+2,k+2;3;t)}{{}_2F_1(k,k;1;t)}\right)\\
&\quad \times \sum_{1\leqslant i<j\leqslant k} z_iz_j + z_{i+k}z_{j+k}\\
&\quad + \left(\frac{(t\log(t))^2k^2\,{}_2F_1(k+1,k+1;2;t)^2}{{}_2F_1(k,k;1;t)^2}\right.\\
&\quad \left. - \frac{t\log(t)^2\,{}_2F_1(k+1,k+1;1;t)}{{}_2F_1(k,k;1;t)}\right)\sum_{1\leqslant i,j\leqslant k} z_iz_{j+k}\\
&\quad + \left(\frac{-(t\log(t))^2k^2\,{}_2F_1(k+1,k+1;2;t)^2}{{}_2F_1(k,k;1;t)^2} + \frac{(t\log(t))^2\binom{k+1}{2}\,{}_2F_1(k+2,k+2;3;t)}{{}_2F_1(k,k;1;t)}\right.\\
&\quad \left. \times \frac{t\log(t)^2k\,{}_2F_1(k+2,k+1;2;t)}{{}_2F_1(k,k;1;t)}\right)\sum_1^{2k}\frac{z_i^2}{2} + \cdots.
\end{aligned} \tag{2.42}$$

Combining the above with (2.29) we have that the first few coefficients B_k in (2.24) are given by

$$\begin{aligned}
B_k(1;) &= \sum_p \frac{k\log(p)}{p-1} - \frac{\log(p)k\,{}_2F_1(k+1,k+1;2;1/p)}{p\,{}_2F_1(k,k;1;1/p)},\\
B_k(1,1;) &= -\sum_p\left(\frac{\log(p)^2k^2\,{}_2F_1(k+1,k+1;2;1/p)^2}{p^2\,{}_2F_1(k,k;1;1/p)^2}\right.\\
&\qquad \left. - \frac{\log(p)^2\binom{k+1}{2}\,{}_2F_1(k+2,k+2;3;1/p)}{p^2\,{}_2F_1(k,k;1;1/p)}\right),\\
B_k(1;1) &= \sum_p \frac{p\log(p)^2}{(p-1)^2} + \left(\frac{\log(p)^2k^2\,{}_2F_1(k+1,k+1;2;1/p)^2}{p^2\,{}_2F_1(k,k;1;1/p)^2}\right.\\
&\qquad \left. - \frac{\log(p)^2{}_2F_1(k+1,k+1;1;1/p)}{p\,{}_2F_1(k,k;1;1/p)}\right),\\
B_k(2;) &= -\sum_p \frac{kp\log(p)^2}{(p-1)^2} + \left(\frac{\log(p)^2k^2\,{}_2F_1(k+1,k+1;2;1/p)^2}{p^2\,{}_2F_1(k,k;1;1/p)^2}\right.
\end{aligned}$$

$$- \frac{\log(p)^2\binom{k+1}{2}\, {}_2F_1(k+2,k+2;3;1/p)}{p^2\, {}_2F_1(k,k;1;1/p)} - \frac{\log(p)^2 k\, {}_2F_1(k+2,k+1;2;1/p)}{p\, {}_2F_1(k,k;1;1/p)}\Bigg). \tag{2.43}$$

2.1.2. Series for the ζ product

Let

$$s\,\zeta(1+s) = 1 + \gamma_0 s - \gamma_1 s^2 + \frac{\gamma_2}{2!}s^3 - \frac{\gamma_3}{3!}s^4 + \cdots \tag{2.44}$$

be the Laurent expansion of $s\zeta(1+s)$ about $s=0$, where the γ_n's generalize Euler's constant

$$\gamma_n = \lim_{m\to\infty}\sum_{k=1}^{m}\frac{\log(k)^n}{k} - \frac{\log(m)^{n+1}}{n+1}. \tag{2.45}$$

As with the series for A_k, we can here exploit the symmetries satisfied by the product

$$\prod_{1\leqslant i,j\leqslant k}(z_i - z_{j+k})\zeta(1+z_i-z_{j+k}). \tag{2.46}$$

We first set $z_{r+1}=\cdots=z_k=0$, $z_{k+r+1}=\cdots=z_{2k}=0$ before applying (2.28), so that (2.46) is equivalent, in its series expansion up to terms involving just $z_1,\dots,z_r$, to

$$\prod_{1\leqslant i,j\leqslant r}(z_i - z_{j+k})\zeta(1+z_i-z_{j+k})\prod_{i=1}^{r}\big(z_i\zeta(1+z_i)\big)^{k-r}\big(-z_{i+k}\zeta(1-z_{i+k})\big)^{k-r}. \tag{2.47}$$

Again, one may use a symbolic differentiation package to evaluate (2.28) applied to the above, and thus obtain the coefficients of the multivariate series expansion

$$\begin{aligned}
&\prod_{1\leqslant i,j\leqslant k}(z_i - z_{j+k})\zeta(1+z_i-z_{j+k}) \\
&\quad = 1 + \gamma k\sum_{1}^{k} z_i - z_{i+k} + \gamma^2 k^2\Bigg(\sum_{1\leqslant i<j\leqslant k} z_i z_j + z_{i+k}z_{j+k}\Bigg) \\
&\qquad + \big(2\gamma_1 + \gamma^2 - \gamma^2 k^2\big)\sum_{1\leqslant i,j\leqslant k} z_i z_{j+k} \\
&\qquad + \big(\gamma^2 k^2 - \gamma^2 k - 2\gamma_1 k\big)\sum_{1}^{2k}\frac{z_i^2}{2} + \cdots.
\end{aligned} \tag{2.48}$$

2.1.3. Multiplying series together

Let us be given two multivariate series of the form that appears, for example, in (2.24)

$$\sum_{\alpha;\beta} C_k(\alpha;\beta)\big(z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k} \pm \mathrm{sym}\big). \tag{2.49}$$

In (2.24) we pulled out the constant term from the series, but generally, the above can have a non-zero constant term $C_k(;)$. The 'sym' indicates that we group together terms with exponents of the same form as explained in the introduction.

We can easily obtain the coefficients of their product by examining, for a given $\alpha;\beta$ the various pairs $\gamma_1;\lambda_1$, $\gamma_2;\lambda_2$ with $\gamma_1+\gamma_2=\alpha$, and $\lambda_1+\lambda_2=\beta$. Some care is needed in carrying this out. While in collecting terms by $C_k(\alpha;\beta)$ we use the conventions in the above paragraph, γ and λ need not satisfy $\gamma \geqslant \lambda$. For example, say with $k=3$, a term of the form $z_1^3 z_2 z_5^2$ can arise through multiplication in 24 ways as $(z_1^{\gamma_{1,1}} z_2^{\gamma_{1,2}} z_3^{\gamma_{1,3}} z_4^{\gamma_{2,1}} z_5^{\gamma_{2,2}} z_6^{\gamma_{2,3}})(z_1^{\lambda_{1,1}} z_2^{\lambda_{1,2}} z_3^{\lambda_{1,3}} z_4^{\lambda_{2,1}} z_5^{\lambda_{2,2}} z_6^{\lambda_{2,3}})$ with $\gamma_{1,1}+\lambda_{1,1}=3$, $\gamma_{1,2}+\lambda_{1,2}=1$, $\gamma_{2,2}+\lambda_{2,2}=2$, and all the others equal to zero. For each of these 24 ways, one needs to look up the corresponding coefficients of both series by sorting the γ and λ and possibly swapping, using (2.23), so that $\gamma \geqslant \lambda$.

In this manner, we are able, given the series for $A_k(z_1,\ldots,z_{2k})$ and the series in (2.48), to obtain the series for the second line in (2.17)

$$\begin{aligned} A_k(z_1,\ldots,z_{2k}) &\prod_{1\leqslant i,j\leqslant k}(z_i-z_{j+k})\zeta(1+z_i-z_{j+k}) \\ &= a_k\sum_{\alpha;\beta} b_k(\alpha;\beta)\big(z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k} \pm \mathrm{sym}\big) \end{aligned} \tag{2.50}$$

(to determine the multivariate series for A_k from that of $\log(A_k(z_1,\ldots,z_{2k}))$, one uses the Taylor series for exp, applied to $\log(A_k)$, and the above multiplication algorithm).

We list the first few terms:

$$\begin{aligned} &A_k(z_1,\ldots,z_{2k}) \prod_{1\leqslant i,j\leqslant k}(z_i-z_{j+k})\zeta(1+z_i-z_{j+k}) \\ &= a_k\Bigg(1+\big(\gamma k + B_k(1;)\big)\sum_1^k z_i - z_{i+k} \\ &\quad + \big(\gamma^2k^2 + B_k(1,1;) + B_k(1;)^2 + 2\gamma k B_k(1;)\big)\sum_{1\leqslant i<j\leqslant k} z_iz_j + z_{i+k}z_{j+k} \\ &\quad + \big(2\gamma_1 + \gamma^2 - \gamma^2k^2 + B_k(1;1) - B_k(1;)^2 - 2\gamma k B_k(1;)\big)\sum_{1\leqslant i,j\leqslant k} z_iz_{j+k} \\ &\quad + \frac{1}{2}\big(\gamma^2k^2 - \gamma^2 k - 2\gamma_1 k + B_k(2;) + B_k(1;)^2 + 2\gamma k B_k(1;)\big)\sum_1^{2k} z_i^2 + \cdots\Bigg). \end{aligned} \tag{2.51}$$

2.2. Determining $c_r(k)$

Extracting the terms of degree r from the Taylor expansion (2.50) and substituting into (2.17) we have

$$\begin{aligned} c_r(k)x^{k^2-r} = {} & \frac{a_k}{k!^2}\frac{1}{(2\pi i)^{2k}}\oint\cdots\oint\frac{\Delta(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_k)\Delta(z_{k+1},\dots,z_{2k})}{\prod_{i=1}^{2k} z_i^{2k}} \\ & \times \sum_{|\alpha|+|\beta|=r} b_k(\alpha;\beta)\big(z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k}\pm \mathrm{sym}\big) \\ & \times e^{\frac{x}{2}\sum_{i=1}^k z_i - z_{i+k}}\,dz_1\dots dz_{2k}. \end{aligned} \tag{2.52}$$

Now, each term in the second line of the integrand with the exponents of the same form integrates the same since the integrand is a symmetric function of $z_1,\dots,z_k$ and of $z_{k+1},\dots,z_{2k}$, and also because the contribution from $z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k}$ is the same as for $z_1^{\beta_1}\cdots z_k^{\beta_k} z_{k+1}^{\alpha_1}\cdots z_{2k}^{\alpha_k}$, as can be seen by changing variables $u_i = -z_i$ and using $b_k(\alpha;\beta) = (-1)^{|\alpha|+|\beta|} b_k(\beta;\alpha)$.

Let $d_k(\alpha;\beta)$ denote the number of terms of a given form of exponent. For example, $d_k(1;) = 2k$ since there are $2k$ terms in $\sum_{i=1}^k z_i - z_{i+k}$. Once can write down a formula for $d_k(\alpha;\beta)$ as, up to a factor of 2, a multinomial coefficient in terms of the multiplicities of the values assumed by the α_i's and β_i's. Let $m_\alpha(j)$ denote the number of occurrences of j amongst $\alpha_1,\dots,\alpha_k$, and likewise for β.

Let J_1 denote the largest value amongst the α_i's and J_2 the largest value amongst the β_i's. Let

$$\delta(\alpha;\beta) = \begin{cases} 1 & \text{if } \alpha = \beta, \\ 0 & \text{if } \alpha \neq \beta. \end{cases} \tag{2.53}$$

We have introduced $\delta(\alpha;\beta)$ to take into account that the $\pm$sym in (2.52) collects together the terms corresponding to $\alpha;\beta$ and to $\beta;\alpha$. We have

$$\begin{aligned} d_k(\alpha;\beta) = {} & 2^{1-\delta(\alpha;\beta)}\binom{k}{m_\alpha(0)}\binom{k-m_\alpha(0)}{m_\alpha(1)} \\ & \times \binom{k-m_\alpha(0)-m_\alpha(1)}{m_\alpha(2)}\cdots\binom{k-m_\alpha(0)\dots-m_\alpha(J_1-1)}{m_\alpha(J_1)} \\ & \times \binom{k}{m_\beta(0)}\binom{k-m_\beta(0)}{m_\beta(1)} \\ & \times \binom{k-m_\beta(0)-m_\beta(1)}{m_\beta(2)}\cdots\binom{k-m_\beta(0)\dots-m_\beta(J_2-1)}{m_\beta(J_2)} \\ = {} & 2^{1-\delta(\alpha;\beta)}(k!)^2\prod_{j=0}^{J_1}\frac{1}{m_\alpha(j)!}\prod_{j=0}^{J_2}\frac{1}{m_\beta(j)!}, \end{aligned} \tag{2.54}$$

since there are $\binom{k}{m_\alpha(0)}$ ways to choose which z_i's, $1 \leqslant i \leqslant k$, have exponent 0, then $\binom{k-m_\alpha(0)}{m_\alpha(1)}$ ways to decide which of the remaining z_i's have exponent 1, etc., and likewise for β. In the simplification to obtain the second line we used $\sum_{j=0}^{J_1} m_\alpha(j) = k$, and similarly for β.

Therefore, counting the number of terms that are collected for a given $b_k(\alpha;\beta)$ we get

$$c_r(k)x^{k^2-r} = \frac{a_k}{k!^2}\frac{1}{(2\pi i)^{2k}}\sum_{|\alpha|+|\beta|=r} b_k(\alpha;\beta)d_k(\alpha;\beta) \times \oint\cdots\oint \frac{\Delta(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_k)\Delta(z_{k+1},\dots,z_{2k})}{\prod_{i=1}^{2k} z_i^{2k}} z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k} \times e^{\frac{x}{2}\sum_{i=1}^k z_i - z_{i+k}}\, dz_1\dots dz_{2k}. \tag{2.55}$$

Pulling out

$$\Delta(z_1,\dots,z_{2k})\Delta(z_1,\dots,z_k)\Delta(z_{k+1},\dots,z_{2k}) \sum_{|\alpha|+|\beta|=r} b_k(\alpha;\beta)d_k(\alpha;\beta) z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k} \tag{2.56}$$

from the integral, we have, as in our consideration of $c_0(k)$,

$$c_r(k) = \frac{a_k}{2^{k^2-r}k!^2} q_2(\partial/\partial x_1,\dots,\partial/\partial x_{2k}) q(\partial/\partial x_1,\dots,\partial/\partial x_{2k}) \prod_1^{2k} \frac{x_i^{2k-1}}{(2k-1)!} \tag{2.57}$$

evaluated at $x_1 = \cdots = x_k = 1$, $x_{k+1} = \cdots = x_{2k} = -1$, where q is given by (2.8) and

$$q_2(z_1,\dots,z_{2k}) = \sum_{|\alpha|+|\beta|=r} b_k(\alpha;\beta)d_k(\alpha;\beta) z_1^{\alpha_1}\cdots z_k^{\alpha_k} z_{k+1}^{\beta_1}\cdots z_{2k}^{\beta_k}. \tag{2.58}$$

As in the proof of Lemma 2.2, (2.57) equals

$$\frac{a_k}{2^{k^2-r}k!^2} q_2(\partial/\partial x_1,\dots,\partial/\partial x_{2k}) \sum_{\mu,\nu} g(\mu,\nu) \tag{2.59}$$

where $g(\mu,\nu)$ equals (2.13) (with $f(x) = x^{2k-1}/(2k-1)!$) and is comprised of a sign and a determinant. The sum is over all $k!^2$ pairs of permutations μ,ν.

Applying $q_2(\partial/\partial x_1,\dots,\partial/\partial x_{2k})$ to these determinants we get

$$\frac{a_k}{2^{k^2-r}} \sum_{|\alpha|+|\beta|=r} \sum_{\mu,\nu} \frac{b_k(\alpha,\beta)d_k(\alpha;\beta)}{k!^2} \operatorname{sgn}(\mu)\operatorname{sgn}(\nu) M_k(\mu,\nu,\alpha,\beta) \tag{2.60}$$

with

$$M_k(\mu,\nu,\alpha,\beta)=\begin{vmatrix} f^{(\mu_1-1+\alpha_1)}(x_1) & f^{(\mu_1+\alpha_1)}(x_1) & \dots & f^{(\mu_1+2k-2+\alpha_1)}(x_1)\\ f^{(\mu_2-1+\alpha_2)}(x_2) & f^{(\mu_2+\alpha_2)}(x_2) & \dots & f^{(\mu_2+2k-2+\alpha_2)}(x_2)\\ \vdots & \vdots & \ddots & \vdots\\ f^{(\mu_k-1+\alpha_k)}(x_k) & f^{(\mu_k+\alpha_k)}(x_k) & \dots & f^{(\mu_k+2k-2+\alpha_k)}(x_k)\\ f^{(\nu_1-1+\beta_1)}(x_{k+1}) & f^{(\nu_1+\beta_1)}(x_{k+1}) & \dots & f^{(\nu_1+2k-2+\beta_1)}(x_{k+1})\\ f^{(\nu_2-1+\beta_2)}(x_{k+2}) & f^{(\nu_2+\beta_2)}(x_{k+2}) & \dots & f^{(\nu_2+2k-2+\beta_2)}(x_{k+2})\\ \vdots & \vdots & \ddots & \vdots\\ f^{(\nu_k-1+\beta_k)}(x_{2k}) & f^{(\nu_k+\beta_k)}(x_{2k}) & \dots & f^{(\nu_k+2k-2+\beta_k)}(x_{2k}) \end{vmatrix}_{2k\times 2k}. \tag{2.61}$$

Setting $x_1=\cdots=x_k=1$, $x_{k+1}=\cdots=x_{2k}=-1$, and rearranging rows (to undo the μ and ν) we get

$$c_r(k)=\frac{a_k}{2^{k^2-r}}\sum_{|\alpha|+|\beta|=r}\sum_{\sigma,\tau}\frac{b_k(\alpha;\beta)d_k(\alpha;\beta)}{k!^2}\tilde{M}_k\big(\sigma(\alpha),\tau(\beta)\big) \tag{2.62}$$

with

$$\tilde{M}_k\big(\sigma(\alpha),\tau(\beta)\big)$$
$$=(-1)^{\sum\beta_i}\begin{vmatrix} \Gamma(2k-\alpha_{\sigma_1})^{-1} & \Gamma(2k-1-\alpha_{\sigma_1})^{-1} & \dots & \Gamma(1-\alpha_{\sigma_1})^{-1}\\ \Gamma(2k-1-\alpha_{\sigma_2})^{-1} & \Gamma(2k-2-\alpha_{\sigma_2})^{-1} & \dots & \Gamma(-\alpha_{\sigma_2})^{-1}\\ \vdots & \vdots & \ddots & \vdots\\ \Gamma(k+1-\alpha_{\sigma_k})^{-1} & \Gamma(k-\alpha_{\sigma_k})^{-1} & \dots & \Gamma(2-k-\alpha_{\sigma_k})^{-1}\\ -\Gamma(2k-\beta_{\tau_1})^{-1} & \Gamma(2k-1-\beta_{\tau_1})^{-1} & \dots & \Gamma(1-\beta_{\tau_1})^{-1}\\ \Gamma(2k-1-\beta_{\tau_2})^{-1} & -\Gamma(2k-2-\beta_{\tau_2})^{-1} & \dots & -\Gamma(-\beta_{\tau_2})^{-1}\\ \vdots & \vdots & \ddots & \vdots\\ (-1)^k\Gamma(k+1-\beta_{\tau_k})^{-1} & (-1)^{k+1}\Gamma(k-\beta_{\tau_k})^{-1} & \dots & (-1)^{3k-1}\Gamma(2-k-\beta_{\tau_k})^{-1} \end{vmatrix}_{2k\times 2k}. \tag{2.63}$$

The extra factor of $(-1)^{\sum\beta_i}$ comes from the extra powers of -1 that are pulled out of the bottom k rows of the matrix. Notice that in order for $\tilde{M}_k$ to be non-zero, the $(\alpha_{\sigma_i}+i-1)$s must be a distinct subset of $\{0,1,2,\dots,2k-1\}$, and similarly for the $(\beta_{\tau_i}+i-1)$s. The implication of this latter point is discussed further in Lemma 2.4 below.

For any α,β, many of the $k!^2$ pairs of permutations σ,τ will give the same determinant because of multiplicity amongst the α_i's and β_i's. In fact, since r is fixed, most of the α_i's and β_i's will equal zero. As before, let $m_\alpha(j)$ denote the number of occurrences of j in $\alpha_1,\dots,\alpha_k$, and similarly for β.

Then (2.62) becomes

$$c_r(k)=\frac{a_k}{2^{k^2-r}}\sum_{|\alpha|+|\beta|=r}\frac{b_k(\alpha;\beta)d_k(\alpha;\beta)}{k!^2}\prod_{j=0}^{J_1}m_\alpha(j)!\prod_{j=0}^{J_2}m_\beta(j)!\sum_{\substack{\text{rearrangements}\\ \sigma,\tau\text{ of }\alpha\text{ and }\beta}}\tilde{M}_k\big(\sigma(\alpha),\tau(\beta)\big). \tag{2.64}$$

By rearrangements, we mean distinct permutations as explained following (1.17). Recall that J_1 and J_2 denote the largest value amongst the α_i's and β_i's respectively.

Notice that this simplifies since, by (2.54),

$$\frac{d_k(\alpha;\beta)}{k!^2}\prod_{j=0}^{J_1} m_\alpha(j)!\prod_{j=0}^{J_2} m_\beta(j)! = 2^{1-\delta(\alpha;\beta)} \tag{2.65}$$

is constant, where $\delta(\alpha;\beta)$ is given by (2.53).

Therefore

$$c_r(k) = \frac{a_k}{2^{k^2-r}}\sum_{|\alpha|+|\beta|=r} 2^{1-\delta(\alpha;\beta)} b_k(\alpha;\beta) \sum_{\substack{\text{rearrangements}\\ \sigma,\tau \text{ of } \alpha \text{ and } \beta}} \tilde{M}_k\big(\sigma(\alpha),\tau(\beta)\big). \tag{2.66}$$

Expression (2.64) can be pared down further by realizing that 'all of the action' takes place in rows $k-|\alpha|+1,\dots,k$ and $2k-|\beta|+1,\dots,2k$. By this we mean that we need only focus on the rearrangements that have $\alpha_{\sigma_1}=\dots=\alpha_{\sigma_{k-|\alpha|}}=0$, and $\beta_{\sigma_1}=\dots=\beta_{\sigma_{k-|\beta|}}=0$, because otherwise the determinant will equal zero.

Lemma 2.4. *The determinant $\tilde{M}_k(\sigma(\alpha),\tau(\beta))$ in* (2.63) *equals zero, unless $\alpha_{\sigma_1}=\dots=\alpha_{\sigma_{k-|\alpha|}}=\beta_{\tau_1}=\dots=\beta_{\tau_{k-|\beta|}}=0$ (in which case it might, or might not, equal zero).*

Proof. Assume that $\tilde{M}_k(\sigma(\alpha),\tau(\beta))\neq 0$. Let $\delta_1 := \alpha_{\sigma_i}\geqslant 1$ be equal to the first non-zero α_σ. But this forces $\delta_2 := \alpha_{\sigma_{i+\delta_1}}$ to also be $\geqslant 1$, otherwise rows i and $i+\delta_1$ would coincide and the determinant would be zero. But then $\delta_3 := \alpha_{\sigma_{i+\delta_1+\delta_2}}$ must also be $\geqslant 1$ otherwise rows $i+\delta_1$ and $i+\delta_1+\delta_2$ would coincide. Continue in this fashion until reaching beyond the kth row, $i+\delta_1+\delta_2+\dots+\delta_j>k$. But, $\delta_1+\dots+\delta_j\leqslant\sum_{m=1}^k \alpha_m=|\alpha|$, so $i+|\alpha|>k$, i.e. $i>k-|\alpha|$. Thus, $\alpha_{\sigma_1}=\dots=\alpha_{\sigma_{k-|\alpha|}}=0$. Similarly, $\beta_{\tau_1}=\dots=\beta_{\tau_{k-|\beta|}}=0$, the only difference in the proof being that the rows would coincide up to a factor of ± 1. □

The above lemma greatly improves the speed with which we can evaluate (2.64) since all but $O_r(1)$ of the terms can be discarded. Consider

$$\frac{1}{2^{k^2-r}}\sum_{\substack{\text{rearrangements}\\ \sigma,\tau \text{ of } \alpha \text{ and } \beta}} \tilde{M}_k\big(\sigma(\alpha),\tau(\beta)\big). \tag{2.67}$$

We will prove in Section 3 using the theory of factorial Schur functions that the above is equal to $\prod_{l=0}^{k-1} l!/(k+l)!$ times a polynomial in k of degree $\leqslant 2(|\alpha|+|\beta|)$, or else is the 0 polynomial.

Hence, if we let $N_k(\alpha;\beta)$ denote the polynomial

$$N_k(\alpha;\beta) = \frac{1}{2^{k^2-r}}\left(\prod_{l=0}^{k-1}\frac{l!}{(k+l)!}\right)^{-1}\sum_{\substack{\text{rearrangements}\\ \sigma,\tau \text{ of } \alpha \text{ and } \beta}} \tilde{M}_k\big(\sigma(\alpha),\tau(\beta)\big) \tag{2.68}$$

we have thus arrived at:

$$c_r(k) = a_k \prod_{l=0}^{k-1} \frac{l!}{(k+l)!} \sum_{|\alpha|+|\beta|=r} 2^{1-\delta(\alpha;\beta)} b_k(\alpha;\beta) N_k(\alpha;\beta). \tag{2.69}$$

The factor $a_k \prod_{l=0}^{k-1} l!/(k+l)!$ is equal to the leading coefficient $c_0(k)$. The $b_k(\alpha,\beta)$'s are the Taylor coefficients of $\frac{1}{a_k} A_k(z_1,\dots,z_{2k}) \prod_{1\leqslant i,j\leqslant k}(z_i - z_{j+k})\zeta(1+z_i-z_{j+k})$, and the first few are listed in (2.51). The function $\delta(\alpha;\beta)$ equals zero unless $\alpha=\beta$ in which case it equals 1. We have thus managed to express $c_r(k)$ as equal to $c_0(k)$ times a polynomial in k with coefficients linear in the $b_k(\alpha,\beta)$'s.

Knowing that $N_k(\alpha;\beta)$ is a polynomial of degree $\leqslant 2(|\alpha|+|\beta|)$ allows us to determine it for a given $\alpha;\beta$ by evaluating (2.68) at $2(|\alpha|+|\beta|)+1$ different values of k and writing the unique polynomial of degree $\leqslant 2(|\alpha|+|\beta|)$ that interpolates those values. Since the arithmetic just involves rational numbers it can be performed exactly. When evaluating the r.h.s. of (2.68) one should make sure to exploit Lemma 2.4 so as to only evaluate $O_r(1)$ of the rearrangements.

In this way, one can find, for example,

$$\begin{aligned} N_k(1;) &= k^2, \\ N_k(2;) &= 0, \\ N_k(1,1;) &= k^2(k-1)(k+1)/2, \\ N_k(1;1) &= -k^2(k-1)(k+1). \end{aligned} \tag{2.70}$$

This allows us to write down formulae for $c_1(k)$ and $c_2(k)$:

$$\begin{aligned} c_1(k) &= \left(a_k \prod_{l=0}^{k-1} \frac{l!}{(k+l)!}\right) 2k^2 b_k(1;) \\ &= \left(a_k \prod_{l=0}^{k-1} \frac{l!}{(k+l)!}\right) 2k^2 \bigl(\gamma k + B_k(1;)\bigr) \end{aligned} \tag{2.71}$$

and, after simplifying,

$$\begin{aligned} c_2(k) &= \left(a_k \prod_{l=0}^{k-1} \frac{l!}{(k+l)!}\right) k^2(k-1)(k+1)\bigl(b_k(1,1;) - b_k(1;1)\bigr) \\ &= \left(a_k \prod_{l=0}^{k-1} \frac{l!}{(k+l)!}\right) k^2(k-1)(k+1) \\ &\quad \times \Bigl(2\bigl(B_k(1;)+\gamma k\bigr)^2 - \gamma^2 - 2\gamma_1 + B_k(1,1;) - B_k(1;1)\Bigr). \end{aligned} \tag{2.72}$$

The B_k's above are given in (2.43). In practice, we were thus able to explicitly determine the first nine lower order terms, $r \leqslant 9$.

3. Proof that $N_k(\alpha;\beta)$ is a polynomial

Throughout this section we use the following notation. Let $e_1, e_2+1, \ldots, e_k+k-1$ be distinct integers and $f_1, f_2+1, \ldots, f_k+k-1$ be distinct integers. If $f_1, f_2+1, \ldots, f_k+k-1$ is a subset of $0, 1, \ldots, 2k-1$, let $c_1, \ldots, c_k$ be the complementary subset. Later we will introduce some extra assumptions on the e_i's and f_i's, namely that most of them are equal to zero.

The following lemma expresses the kind of $2k \times 2k$ determinant that appears in the formula for N_k as a $k \times k$ determinant involving binomial coefficients.

Lemma 3.1. *Let e_i and f_i be given as above. Then*

$$\left|\begin{matrix} \Gamma(2k-e_1)^{-1} & \Gamma(2k-1-e_1)^{-1} & \ldots & \Gamma(1-e_1)^{-1} \\ \Gamma(2k-1-e_2)^{-1} & \Gamma(2k-2-e_2)^{-1} & \ldots & \Gamma(-e_2)^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ \Gamma(k+1-e_k)^{-1} & \Gamma(k-e_k)^{-1} & \ldots & \Gamma(2-k-e_k)^{-1} \\ -\Gamma(2k-f_1)^{-1} & \Gamma(2k-1-f_1)^{-1} & \ldots & \Gamma(1-f_1)^{-1} \\ \Gamma(2k-1-f_2)^{-1} & -\Gamma(2k-2-f_2)^{-1} & \ldots & -\Gamma(-f_2)^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ (-1)^k\Gamma(k+1-f_k)^{-1} & (-1)^{k+1}\Gamma(k-f_k)^{-1} & \ldots & (-1)^{3k-1}\Gamma(2-k-f_k)^{-1} \end{matrix}\right|_{2k\times 2k}$$

$$= \operatorname{sgn}(f)\left(\prod_{l=0}^{k-1}\frac{(e_{l+1}+l)!(f_{l+1}+l)!}{l!(k+l)!}2^{c_{l+1}-e_{l+1}-l}\right)\left|\binom{c_j}{e_i+i-1}\right|_{k\times k}, \tag{3.1}$$

where $\operatorname{sgn}(f)$ is (-1) raised to the number of transpositions needed to get f_1+1, $f_2+2, \ldots, f_k+k$ sorted into increasing numerical order.

Also note, if e_i's and f_i's are not distinct as required, then two of the rows on the l.h.s. will coincide up to sign, and hence the determinant will equal zero.

Proof. Introducing a $(2k-j)!$ in column j, $1/(e_i+i-1)!$ in row i and $(-1)^{i-1}/(f_i+i-1)!$ in row $k+i$, $i=1,\ldots,k$, the l.h.s. of (3.1) equals

$$(-1)^{\frac{(k-1)k}{2}}\prod_{l=0}^{k-1}\frac{(e_{l+1}+l)!(f_{l+1}+l)!}{l!(k+l)!}\left|\begin{matrix} \binom{2k-1}{e_1} & \binom{2k-2}{e_1} & \ldots & \binom{0}{e_1} \\ \binom{2k-1}{e_2+1} & \binom{2k-2}{e_2+1} & \ldots & \binom{0}{e_2+1} \\ \vdots & \vdots & \ddots & \vdots \\ \binom{2k-1}{e_k+k-1} & \binom{2k-2}{e_k+k-1} & \ldots & \binom{0}{e_k+k-1} \\ -\binom{2k-1}{f_1} & +\binom{2k-2}{f_1} & \ldots & +\binom{0}{f_1} \\ -\binom{2k-1}{f_2+1} & +\binom{2k-2}{f_2+1} & \ldots & +\binom{0}{f_2+1} \\ \vdots & \vdots & \ddots & \vdots \\ -\binom{2k-1}{f_k+k-1} & +\binom{2k-2}{f_k+k-1} & \ldots & +\binom{0}{f_k+k-1} \end{matrix}\right|_{2k\times 2k}. \tag{3.2}$$

Multiplying the matrix in (3.2) on the right by a unit, i.e. by

$$\left|\binom{j-1}{2k-i}\right|_{2k\times 2k} = (-1)^k \tag{3.3}$$

the ij entry is, for $1 \leqslant i \leqslant k$, $1 \leqslant j \leqslant 2k$,

$$\sum_{m=0}^{2k-1} \binom{m}{e_i+i-1}\binom{j-1}{m} = 2^{j-e_i-i}\binom{j-1}{e_i+i-1}, \tag{3.4}$$

and the $(i+k)j$ entry is, for $1 \leqslant i \leqslant k$, $1 \leqslant j \leqslant 2k$,

$$\sum_{m=0}^{2k-1} \binom{m}{f_i+i-1}\binom{j-1}{m}(-1)^m = \begin{cases} (-1)^{f_i+i-1} & \text{if } j = f_i+i, \\ 0 & \text{otherwise.} \end{cases} \tag{3.5}$$

These binomial identities can be proven by noticing that $\binom{m}{A}\binom{B}{m} = \binom{B}{A}\binom{B-A}{m-A}$ and using the binomial theorem.

Expanding the determinant of this new matrix along the last k rows, and pulling out powers of 2's from the first k rows gives the lemma. The $\operatorname{sgn}(f)$ that appears in the lemma can be obtained as follows. The last k rows of the matrix given by (3.4) and (3.5) consist of ± 1's with a $(-1)^{f_i+i-1}$ appearing in row $k+i$ and column f_i+i, $1 \leqslant i \leqslant k$. We can swap the columns and rows of this matrix so that the bottom left $k \times k$ submatrix becomes diagonal, and the lower right submatrix becomes, $0_{k\times k}$, the zero submatrix.

There are many ways to do so, but to end up with the determinant in the lemma, one should make sure that we do not rearrange the relative ordering of the columns corresponding to $c_1, \dots, c_k$. If the quantities $f_i + i$ appear in increasing numerical value, one can simply swap column $f_i + i$ with its neighboring columns on the left, one at a time, until it sits in the ith column. This introduces a $(-1)^{\sum_{i=1}^k f_i}$ into the determinant.

However, if the $(f_i + i)$s appear out of order, in order to preserve the ordering of the columns corresponding to $c_1, \dots, c_k$, one should first swap rows so as to put the lower $k \times 2k$ submatrix into reduced row echelon form. For example if one has $f_{i_1} + i_1 > f_{i_2} + i_2$, but $i_1 < i_2$ then one should swap rows $k + i_1$ and $k + i_2$. This has the effect of placing the $(-1)^{f_{i_1}+i_1-1}$ in entry $(i_2, f_{i_1} + i_1) = (i_2, (f_{i_1} + i_1 - i_2) + i_2)$, and the $(-1)^{f_{i_2}+i_2-1}$ in entry $(i_1, f_{i_2} + i_2) = (i_1, (f_{i_2} + i_2 - i_1) + i_1)$. The horizontal displacement then needed to get these entries into the i_2nd and i_1st columns is therefore unchanged and equal to $f_{i_1} + f_{i_2}$. Relabeling and repeating if necessary, one sees that the contribution to the determinant from the row and column swaps that get the lower left $k \times k$ submatrix into diagonal form is

$$(-1)^{\operatorname{sgn}(f)+\sum f_i}, \tag{3.6}$$

where $\operatorname{sgn}(f)$ accounts for the number of transpositions needed to get $f_1 + 1, \dots, f_k + k$ into increasing numerical order.

One now easily evaluates the determinant by expanding along the lower diagonal matrix. This submatrix begins at entry $k+1$, 1 and this contributes a $(-1)^k$ to the determinant. One also needs to multiply the diagonal entries themselves, and this contributes a $(-1)^{\sum f_i+i-1}$.

Collecting the powers of -1 that appear in (3.2) and (3.3) and multiplying by (3.6) and by the two factors in the previous paragraph we obtain the sign that appears in the lemma. □

Now (3.1) equals

$$(-1)^{k(k-1)/2}\operatorname{sgn}(f)\prod_{l=0}^{k-1}\frac{(f_{l+1}+l)!}{l!(k+l)!}2^{c_{l+1}-e_{l+1}-l}\left|(c_i)_{\lambda_j+k-j}\right|_{k\times k} \tag{3.7}$$

with $(z)_\mu = z(z-1)\dots(z-\mu+1)$ the *descending* factorial, and $\lambda_j = e_{k-j+1}$. The determinant above is essentially a factorial Schur function.

We have introduced the λ_j's and taken the transpose so as to conveniently apply theorems of MacDonald and Chen–Louck (see [CL, Theorems 3.2, 3.3]) concerning the factorial Schur function. The extra $(-1)^{k(k-1)/2}$ above comes from swapping the i, j entry with the $i, k-j+1$ entry.

In our application to $N_k(\alpha;\beta)$, we found, in Lemma 2.4, that most terms in (2.68) can be discarded, and only terms with $\alpha_{\sigma_1} = \dots = \alpha_{\sigma_{k-|\alpha|}} = \beta_{\tau_1} = \dots = \beta_{\tau_{k-|\beta|}} = 0$ contribute.

So assume that, for some $s \geqslant 0$, $e_1 = \dots = e_{k-s} = 0$, and hence $\lambda_{s+1} = \dots = \lambda_k = 0$. Next, write $c_j = k+j-1-\epsilon_j$, where ϵ_j is a non-negative integer. Assume that, for some $t \geqslant 0$, $\epsilon_j = 0$ for all $j > t$, i.e. that $c_j = k+j-1$, if $j > t$.

To apply their theorems, one must first assume that the λ_j's are decreasing $\lambda_1 \geqslant \lambda_2 \geqslant \cdots$. We can assume this condition by rearranging the first s columns of the matrix in (3.7) if necessary. This will change the sign of the determinant by a power of (-1) that depends only on $\lambda_1, \dots, \lambda_s$. However, since we are actually permuting the $(\lambda_j + k - j)$s rather than the λ_j's, some care is needed.

Say $\lambda_j < \lambda_{j+1}$. We are assuming that the $(\lambda_j + k - j)$s are distinct (we have assumed the $(e_j + j - 1)$s to be distinct), thus $\lambda_j < \lambda_{j+1}$ actually implies that

$$\lambda_j < \lambda_{j+1} - 1 \tag{3.8}$$

since otherwise one would have two neighboring $(\lambda_j + k - j)$s that were equal.

Swapping columns j and $j+1$, the subscript for the jth column is then $\lambda_{j+1} + k - j - 1 = (\lambda_{j+1} - 1) + k - j$, and for the $(j+1)$st column is then $\lambda_j + k - j = (\lambda_j + 1) + k - j - 1$. Therefore we have replaced $(\lambda_1, \dots, \lambda_j, \lambda_{j+1}, \dots)$ with $(\lambda_1, \dots, \lambda_{j+1} - 1, \lambda_j + 1, \dots)$ in which $\lambda_{j+1} - 1 \geqslant \lambda_j + 1$. Also notice that swapping the two columns only permutes the subscripts which therefore remain distinct.

Continuing in this fashion, we end up with $\tilde\lambda_1 \geqslant \dots \geqslant \tilde\lambda_s$, with the $\tilde\lambda_i$ obtained from the λ_i's by the above swapping procedure. Notice that

$$\sum \tilde\lambda_i = \sum \lambda_i \tag{3.9}$$

since each swap adds one and subtracts one from the λ_i's.

Theorem 3.2. *Assume that $c_j = k + j - 1 - \epsilon_j$, with $\epsilon_j = 0$ if $j > t$, that $\tilde\lambda_1 \geqslant \tilde\lambda_2 \geqslant \dots \geqslant \tilde\lambda_s$ and that $\tilde\lambda_{s+1} = \dots = \tilde\lambda_k = 0$. Then*

$$\left|(c_i)_{\tilde\lambda_j+k-j}\right|_{k\times k} = (-1)^{k(k-1)/2}\Delta(c) \times \Big(\textit{polynomial in } k \textit{ of degree} \leqslant 2\sum \tilde\lambda_i\Big). \tag{3.10}$$

Proof. By [CL, Theorems 3.2, 3.3, and p. 4150] one has

$$\left|(c_i)_{\tilde{\lambda}_j+k-j}\right|_{k\times k} = (-1)^{k(k-1)/2}\Delta(c)\left|w_{\tilde{\lambda}_i-i+j}(c+j-1)\right|_{k\times k} \tag{3.11}$$

with $c+j-1=(c_1+j-1,\dots,c_k+j-1)$, $\Delta(c)=\prod_{1\leqslant i<j\leqslant m}(c_j-c_i)$, and

$$w_m(z) = \sum_{i_1\leqslant\cdots\leqslant i_m\leqslant k} y_{i_1}(y_{i_2}-1)\cdots(y_{i_m}-m+1) \tag{3.12}$$

with $y_i = z_i - i + 1$ and the conventions that $w_0(z)=1$, and $w_m(z)=0$ if $m<0$. The main point is that our $k\times k$ determinant has been replaced by an $s\times s$ determinant. Furthermore,

$$w_m(c+j-1) = \sum_{i_1\leqslant\cdots\leqslant i_m\leqslant k} (k+j-1-\epsilon_{i_1})(k+j-2-\epsilon_{i_2})\cdots(k+j-m-\epsilon_{i_m}). \tag{3.13}$$

The terms in this sum with all i's $>t$ contribute

$$\binom{k-t}{m}(k+j-1)\cdots(k+j-m)$$

since $\epsilon_i = 0$ if $i>t$. This is a polynomial of degree $2m$ in k.

The terms with $i_1\leqslant t$ and the other i's $>t$ contribute

$$\binom{k-t}{m-1}(k+j-2)\cdots(k+j-m)\sum_{i_1=1}^{t}(k+j-1-\epsilon_{i_1}),$$

and the terms with $i_1\leqslant i_2\leqslant t$ contribute

$$\binom{k-t}{m-2}(k+j-3)\cdots(k+j-m)\sum_{1\leqslant i_1\leqslant i_2\leqslant t}(k+j-1-\epsilon_{i_1})(k+j-2-\epsilon_{i_2}),$$

both of which are polynomials in k of degree $2m-1$ and $2m-2$ respectively. In this fashion one sees that the entries of

$$\left|w_{\tilde{\lambda}_i-i+j}(c+j-1)\right|_{s\times s}$$

are polynomials in k. Furthermore, expanding this determinant we get a sum of products of entries, one from each row and column. However, $w_m(z)=0$ if $m<0$, so only the terms with all $\tilde{\lambda}_i - i + j \geqslant 0$ contribute, and the degree of such a term is then $2\sum\tilde{\lambda}_i$. □

Applying Theorem 3.2 we find that (3.7) equals

$$\Delta(c)\prod_{l=0}^{k-1}\frac{(f_{l+1}+l)!}{l!(k+l)!}2^{c_{l+1}-e_{l+1}-l}\times\left(\text{polynomial in } k \text{ of degree} \leqslant 2\sum\lambda_i\right). \tag{3.14}$$

Here we have absorbed the factor of ±1 into the polynomial and have also used (3.9).

Thus, given that $\alpha_{\sigma_1}, \alpha_{\sigma_2}+1, \ldots, \alpha_{\sigma_k}+k-1$ are distinct and $\beta_{\tau_1}, \beta_{\tau_2}+1, \ldots, \beta_{\tau_k}+k-1$ are distinct, we get that a typical $\tilde{M}_k(\sigma(\alpha), \tau(\beta))$ appearing in (2.68) equals:

$$\tilde{M}_k\bigl(\sigma(\alpha), \tau(\beta)\bigr) = \Delta(\gamma) \prod_{l=0}^{k-1} \frac{(\beta_{\tau_{l+1}}+l)!}{l!(k+l)!} 2^{\gamma_{l+1}-\alpha_{\sigma_{l+1}}-l} \times \bigl(\text{polynomial in } k \text{ of degree} \leqslant 2|\alpha|\bigr) \tag{3.15}$$

where γ is the complementary subset of the $(\beta_{\tau_i}+i-1)$s.

$$\{\gamma_1, \ldots, \gamma_k\} = \{0, 1, \ldots, 2k-1\} - \{\beta_{\tau_1}, \beta_{\tau_2}+1, \ldots, \beta_{\tau_k}+k-1\} \tag{3.16}$$

and $\Delta(\gamma) = \prod_{i<j}(\gamma_j - \gamma_i)$.

Now, by Lemma 2.4, most of the α_{σ_i}'s and β_{τ_i}'s are 0,

$$\alpha_{\sigma_1} = \cdots = \alpha_{\sigma_{k-|\alpha|}} = \beta_{\tau_1} = \cdots = \beta_{\tau_{k-|\beta|}} = 0, \tag{3.17}$$

and $\gamma_j = k + j - 1 - \epsilon_j$ where $\epsilon_j = 0$ if $j > |\beta|$. The latter can be seen by noticing that $\beta_{\tau_i} + i - 1 \leqslant |\beta| + k - 1$ so that $\{k + |\beta|, \ldots, 2k-1\}$ is a subset of γ. Thus, starting from the end, $\epsilon_k = 0$, hence $\epsilon_{k-1} = 0, \ldots, \epsilon_{|\beta|+1} = 0$.

Hence,

$$\Delta(\gamma) = \prod_{1 \leqslant i<j \leqslant k} (j - i + \epsilon_i - \epsilon_j) = \prod_{1 \leqslant i<j \leqslant k} (j-i) \prod_{1 \leqslant i<j \leqslant k} \left(1 + \frac{\epsilon_i - \epsilon_j}{j-i}\right). \tag{3.18}$$

The first product gives

$$\prod_{l=1}^{k} l! \tag{3.19}$$

and, because $\epsilon_i = \epsilon_j = 0$ if $i, j > |\beta|$ the second factor equals

$$\prod_{1 \leqslant i<j \leqslant |\beta|} \left(1 + \frac{\epsilon_i - \epsilon_j}{j-i}\right) \prod_{\substack{1 \leqslant i \leqslant |\beta| \\ |\beta| < j \leqslant k}} \frac{j - i + \epsilon_i}{j-i}. \tag{3.20}$$

However, the product over $1 \leqslant i < j \leqslant |\beta|$ is a rational number. Furthermore, most of the numerator of the product over $1 \leqslant i \leqslant |\beta|$, $|\beta| < j \leqslant k$ cancels with the denominator leaving a polynomial in k of degree $|\epsilon|$.

But $|\beta| = |\epsilon|$ which is easily verified as follows. The union of the $(\beta_i + i - 1)$s and γ_i's give $\{0, 1, \ldots, 2k-1\}$, so

$$\sum_{i=1}^{k} \beta_i + i - 1 + \gamma_i = \sum_{i=0}^{2k-1} i. \tag{3.21}$$

Substituting $\gamma_i = k + i - 1 - \epsilon_i$ and simplifying gives $\sum \beta_i = \sum \epsilon_i$.

Collecting the above together gives

$$\Delta(\gamma) = \prod_{l=1}^{k} l! \times \bigl(\text{polynomial in } k \text{ of degree } |\beta|\bigr) \tag{3.22}$$

(we take the polynomial to be 1 if $|\beta| = 0$).

Next, we determine the power of 2 appearing in (3.15):

$$\sum_{l=0}^{k} \gamma_{l+1} - \alpha_{\sigma_{l+1}} - l = \sum_{l=0}^{k} k + l - \epsilon_{l+1} - \alpha_{\sigma_{l+1}} - l = k^2 + |\beta| - |\alpha|. \tag{3.23}$$

Finally,

$$\prod_{l=0}^{k-1} \frac{(\beta_{\tau_{l+1}} + l)!}{l!} = \text{polynomial in } k \text{ of degree } |\beta|, \tag{3.24}$$

because $\beta_{\tau_1} = \cdots = \beta_{\tau_{k-|\beta|}} = 0$, and where we regard the l.h.s. as a function of k with $\beta_{\tau_{k-j}}$ fixed for $0 \leqslant j \leqslant |\beta|$. Therefore, most of the numerator cancels with the denominator except for $|\beta|$ factors each of which is a polynomial of degree 1 in k. We have therefore shown that

$$\tilde{M}_k\bigl(\sigma(\alpha), \tau(\beta)\bigr) = 2^{k^2} \prod_{l=0}^{k} \frac{l!}{(k+l)!} \times \bigl(\text{polynomial in } k \text{ of degree} \leqslant 2\bigl(|\alpha| + |\beta|\bigr)\bigr). \tag{3.25}$$

Here we have absorbed the extra $2^{|\beta|-|\alpha|}$ from (3.23) into the polynomial. This proves that $N_k(\alpha; \beta)$ given by (2.68) is a polynomial in k of degree $\leqslant 2(|\alpha| + |\beta|)$.

4. Numerical evaluation of $c_r(k)$

Two methods were developed to numerically compute the coefficients $c_r(k)$ of the lower order terms. The first relied on (2.69) and we used Maple [M] to take advantage of its symbolic capabilities. This approach had the advantage of allowing us to obtain the coefficients to many digits precision, and also to make sense of the conjecture for non-integer values of k. This method suffered the disadvantage of being difficult to implement, even using a high level symbolic package, and required much computational power, so that we only determined $c_r(k)$ in this way up to $r \leqslant 9$. This sufficed to compute all the lower terms, for $k = 3$, since $P_k(x) = c_0(k)x^{k^2} + c_1(k)x^{k^2-1} + \cdots + c_{k^2}(k)$ is a polynomial in x of degree k^2.

The second method was comparatively easy to implement, and allowed us to obtain many more coefficients. However, it is limited to integer values of k, and also presents more difficulties in acceleration therefore yielding lower precision.

4.1. Method 1

A table of the polynomials $N_k(\alpha;\beta)$ of degree $\leqslant 2(|\alpha|+|\beta|)$ was prepared by evaluating (2.68) at slightly more than $2(|\alpha|+|\beta|)+1$ values of k and interpolating the unique polynomial of said degree fitting those points. The extra points were thrown in for good measure as a check against errors. This was done for all $0 \leqslant |\alpha|+|\beta| \leqslant 9$.

Next a corresponding table of the coefficients $b_k(\alpha;\beta)$ was prepared, expressed symbolically as a polynomial in the γ_j's and $B_k(\alpha;\beta)$'s as described in Section 2.1, with $B_k(\alpha;\beta)$ given as a sum over primes, with the summand equal to $\log(p)^{|\alpha|+|\beta|}$ times a function rational in p and in Gauss hypergeometric functions of the form ${}_2F_1(k+A,k+B;C;1/p)$, where A,B,C are non-negative integers, $C \geqslant 1$. A few example $B_k(\alpha;\beta)$'s are listed in (2.43).

We were then able to obtain, for a given k, numerical values of the coefficients $c_r(k)$, for $0 \leqslant r \leqslant 9$. Because $B_k(\alpha;\beta)$ is expressed as an infinite sum over primes, we used standard methods to accelerate its convergence. Namely, we evaluated the first few terms, $p \leqslant P$, to high precision. Then, to evaluate the tail end of the sum, $p > P$, we used Maple's series routine to determined the first few terms of the series expansion in $1/p$ of the summand, writing it in the form

$$(\log p)^r \sum_{j=2}^{6} \frac{d_j}{p^j} \tag{4.1}$$

where $r = |\alpha|+|\beta|$, and the d_j's depend on the summand hence on α and β.

To evaluate a sum of the form

$$\sum_{p>P} \frac{\log(p)^r}{p^j} \tag{4.2}$$

we first wrote it as a full sum minus the front end:

$$\sum_{p} \frac{\log(p)^r}{p^j} - \sum_{p\leqslant P} \frac{\log(p)^r}{p^j}. \tag{4.3}$$

The second sum was evaluated by summing the terms $p \leqslant P$, while first sum was computed using Mobius inversion:

$$\log\zeta(s) = \sum_{m=1}^{\infty} \frac{1}{m} \sum_{p} \frac{1}{p^{ms}}, \quad \Re(s) > 1, \tag{4.4}$$

so

$$\sum_{p} \frac{1}{p^s} = \sum_{m=1}^{\infty} \frac{\mu(m)}{m} \log\zeta(ms), \tag{4.5}$$

and hence

$$\sum_p \frac{\log(p)^r}{p^s} = (-1)^r \sum_{m=1}^{\infty} \frac{\mu(m)}{m} \big(\log\zeta(ms)\big)^{(r)}. \tag{4.6}$$

Now $(\log\zeta(ms))^{(r)}$ decreases exponentially fast in m, as can be seen by considering its Dirichlet series which is dominated by the first term, and only a handful of m on the r.h.s. of (4.6) are needed to evaluate $\sum_p \frac{\log(p)^r}{p^s}$ to a given precision.

The factor a_k given by (1.7) can be evaluated to high precision in a similar way.

In this manner we were able to compute $c_r(k)$, $0 \leqslant r \leqslant 9$ for various k. For example, for $k=3$ we obtained the coefficients to about 30 decimal places. The actual precision can be predicted from the size of P, as the overall error in using (4.1) to approximate the summand for the terms $p > P$ is $O(\log(P)^{r-1}/P^6)$. In practice, we took larger and larger values of P until the numerics stabilized to a precision that we found satisfying.

4.2. *Method 2*

The second method we developed to compute $c_r(k)$ used the combinatorial sum (1.11), small shifts, and very high precision to capture cancellation amongst the high order poles of the terms in the sum. Because this method requires very little symbolically, this was implemented in `C++` using NTL [S] to carry out multiprecision arithmetic.

The basic idea is as follows. The polynomial $P_k(x)$ given by (1.2) can be regarded as a special case of the function $P_k(\alpha, x)$ given by (1.10), namely with $\alpha_1 = \cdots = \alpha_{2k} = 0$. One can then use (1.11) to evaluate $P_k(\alpha, x)$. However, the terms in (1.11) have poles if the α_i's are not distinct. So, we cannot simply substitute $\alpha = \mathbf{0}$ and sum the terms numerically. Instead we take the limit as $\alpha \to \mathbf{0}$ with the condition that the α_i's are distinct. One must also use very high precision to capture cancellation amongst the terms which individually become very large when α is small.

More precisely, let

$$H(z_1, \ldots, z_{2k}; x) = \exp\left(\frac{x}{2}\sum_1^k z_j - z_{j+k}\right) A_k(z_1, \ldots, z_{2k}) \prod_{i=1}^k \prod_{j=1}^k \zeta(1 + z_i - z_{j+k}), \tag{4.7}$$

and let $\epsilon_j = j\epsilon$, where $\epsilon \in \mathbb{C}$. Then, by (1.11)

$$P_k(x) = \lim_{\epsilon \to 0} \sum_{\sigma \in \Xi} H(\epsilon_{\sigma(1)}, \ldots, \epsilon_{\sigma(2k)}; x), \tag{4.8}$$

where Ξ is the set of $\binom{2k}{k}$ permutations $\sigma \in S_{2k}$ such that $\sigma(1) < \cdots < \sigma(k)$ and $\sigma(k+1) < \cdots < \sigma(2k)$.

Therefore, expanding exp in its Taylor series, and pulling out the coefficient of x^{k^2-r}, we get

$$c_r(k) = \frac{1}{2^{k^2-r}(k^2-r)!} \lim_{\epsilon \to 0} \sum_{\sigma \in \Xi} H_r(\epsilon_{\sigma(1)}, \ldots, \epsilon_{\sigma(2k)}), \tag{4.9}$$

where

$$H_r(z_1, \ldots, z_{2k}) = \left(\sum_1^k z_j - z_{j+k}\right)^{k^2-r} A_k(z_1, \ldots, z_{2k}) \prod_{i=1}^k \prod_{j=1}^k \zeta(1 + z_i - z_{j+k}). \tag{4.10}$$

The only complication in evaluating the above for a given k and ϵ is that $A_k(z_1,\dots,z_{2k})$ is expressed as an infinite product over primes (1.4). To evaluate that product, we broke it up into $p \leqslant P$ and $p > P$, with P large. For the primes $p \leqslant P$, we used (1.5) to evaluate the contribution from p, each factor only requiring finitely many arithmetic steps.

For the contribution from the larger primes, $p > P$, we used a quadratic approximation for the local factor appearing in (1.4):

$$1-\sum_{\substack{1\leqslant i_1<i_2\leqslant k\\ 1\leqslant j_1<j_2\leqslant k}} p^{-2-z_{i_1}-z_{i_2}+z_{k+j_1}+z_{k+j_2}}. \tag{4.11}$$

This approximation can be obtained by substituting $u_j = p^{-1/2-z_j}$ and $w_j = p^{-1/2+z_{k+j}}$ in the local factor of (1.4), and working out the terms up to degree four. Only terms of even degree appear because the integral over θ pulls out just the terms with the same number of u's and w's. So, we expand each geometric series appearing in the integral over θ up to degree two, multiply them out, and collect terms with the same number of u's and w's.

The first factor $\prod(1-u_i w_j)$ appears precisely to cancel the terms of degree two in the second factor, so we need only determine the terms of degree four. Noticing that the local factor is symmetric separately in the u's and w's, and also if we swap u and w, we can determine the terms of degree four by simply computing all representative fourth order partial derivatives that have the same number of u's as w's, evaluated at $u_j = w_j = 0$, $1 \leqslant j \leqslant k$. For instance, it is enough to immediately set $u_j = w_j = 0$ if $3 \leqslant j \leqslant k$ and then take the partial derivatives: $\frac{\partial}{\partial u_1}\frac{\partial}{\partial u_2}\frac{\partial}{\partial w_1}\frac{\partial}{\partial w_2}$, $\frac{\partial}{\partial u_1}\frac{\partial}{\partial u_2}\frac{\partial^2}{\partial w_1^2}$, $\frac{\partial^2}{\partial u_1^2}\frac{\partial^2}{\partial w_1^2}$, evaluated at $u_1 = u_2 = w_1 = w_2 = 0$. Doing so gives that the local factor, up to terms of degree four, equals

$$1-\sum_{\substack{1\leqslant i_1<i_2\leqslant k\\ 1\leqslant j_1<j_2\leqslant k}} u_{i_1}u_{i_2}w_{j_1}w_{j_2}, \tag{4.12}$$

thus giving (4.11).

Therefore, we used

$$\begin{aligned}&\prod_{p>P}\prod_{\substack{1\leqslant i_1<i_2\leqslant k\\ 1\leqslant j_1<j_2\leqslant k}}\left(1-p^{-2-z_{i_1}-z_{i_2}+z_{k+j_1}+z_{k+j_2}}\right)\\ &\quad=\frac{\prod_{\substack{1\leqslant i_1<i_2\leqslant k\\ 1\leqslant j_1<j_2\leqslant k}}\zeta(2+z_{i_1}+z_{i_2}-z_{k+j_1}-z_{k+j_2})^{-1}}{\prod_{p\leqslant P}\prod_{\substack{1\leqslant i_1<i_2\leqslant k\\ 1\leqslant j_1<j_2\leqslant k}}(1-p^{-2-z_{i_1}-z_{i_2}+z_{k+j_1}+z_{k+j_2}})}\end{aligned} \tag{4.13}$$

to approximate the contribution to (1.4) for the primes $p > P$.

To compute (4.9) to D decimal places, we should take ϵ roughly of size 10^{-D} and then use about $(r+1)D$ digits working precision to account for cancellation in (4.9) amongst the order r pole in ϵ of the summands. Since r can be as large as k^2, we used $(k^2+8)D$ digits working precision, the $+8$ taken for extra leeway, and also chose D to be slightly larger than the desired final precision.

5. Verifying the full moment conjecture

In [CFKRS] we presented numerical data supporting the conjecture described in Section 1.1 for $k = 3$. Here we give some more data supporting the conjecture, for integer $k \leqslant 7$, and also for several real and complex values of k. Our data supports the conjecture, but is not too extensive as our main effort was put towards developing ways to evaluate the lower terms rather than to large scale verification of the conjecture. Nonetheless, even moderate data strongly supports the conjecture.

One experiment we carried out involved comparing the two quantities

$$\int_C^D \left|\zeta\left(\frac{1}{2} + it\right)\right|^{2k} dt \tag{5.1}$$

and

$$\int_C^D P_k\big(\log(t/2\pi)\big)\, dt, \tag{5.2}$$

for seventeen intervals $[C, D]$ of length 50 000, and $k = 3, 4, 5, 6,$ and 7. We also examined the conjecture for several non-integer values of k, in the latter case interpreting $P_k(x)$ as an asymptotic series rather than as polynomial.

For both integer and non-integer k, we used Method 1 of Section 4.1 to compute the first few lower terms to high precision. For $k = 3, 4, 5, 6, 7, 8$ we also computed $c_r(k)$ for $r \leqslant k^2$ using Method 2.

Tables of the coefficients $c_r(k)$, $k = 3, 4, 5, 6, 7$ can be found in [CFKRS]. As k increases, it seems from numerics that the first few leading order terms have much smaller coefficients than the later lower order terms. For example, when $k = 4$, the leading term as listed in [CFKRS] is $c_0(4) = 0.24650183919342276 \times 10^{-12}$, compared to the largest value $c_{13}(4) = 38.203306$. To verify the full moment conjecture, we needed to evaluate $P_k(x)$ at $x = \log(t/(2\pi))$. Therefore, even if t is moderately large, say 10^6, the main contribution actually comes from substantially lower order terms. In the range we examined, the main contribution for $k = 3, 4, 5, 6, 7$ came, respectively, from the terms $r = 3, 6, 12, 20, 30$ and their immediate neighbors.

To compare to actual moment data for ζ we used Mathematica [Ma] to numerically integrate powers of $|\zeta(1/2 + it)|$ for each interval. Due the oscillatory nature of ζ, we performed the integration between consecutive zeros of ζ on the half-line using a table of zeros computed with the L-function calculator [R].

Tables 1 and 2 gives the values of (5.2) and (5.1) for $[C, D] = [50\,000n, 50\,000(n + 1)]$, $n = 0, 1, \dots, 16$, and $k = 3, 4, 5, 6, 7$. The data for $k = 3$ is a subset of the data given in [CFKRS], but otherwise, the data here is new. We see that the pairs of columns track one another nicely.

Figure 1 depicts the difference between (5.2) and (5.1) divided by (5.1) for the values in Tables 1 and 2.

We also present some data for non-integer k, specifically for $k = 0.5, 1.8, 3.2,$ and $0.5 + i$ taking just the first few terms, $r \leqslant 7$, of $P_k(x)$. For non-integer k we believe, based on our numerics, that $P_k(x)$, no longer a polynomial in x but an infinite series, gives an asymptotic

Table 1
This table compares the conjectured value (5.2) to actual data (5.1) for intervals $[50\,000n, 50\,000(n+1)]$, $n = 0, 1, \ldots, 16$, and $k = 3, 4, 5$. The fit is to two or three decimal places, consistent with the remainder stated in (1.1)

n	conj. $k=3$	data $k=3$	conj. $k=4$	data $k=4$	conj. $k=5$	data $k=5$
0	7.23687×10^{9}	7.23101×10^{9}	1.89527×10^{12}	1.88501×10^{12}	6.00428×10^{14}	5.91051×10^{14}
1	1.56965×10^{10}	1.57239×10^{10}	5.67575×10^{12}	5.70833×10^{12}	2.45298×10^{15}	2.47886×10^{15}
2	2.15687×10^{10}	2.15368×10^{10}	9.17127×10^{12}	9.12987×10^{12}	4.68619×10^{15}	4.64908×10^{15}
3	2.63814×10^{10}	2.62463×10^{10}	1.24573×10^{13}	1.23432×10^{13}	7.10198×10^{15}	7.04187×10^{15}
4	3.05562×10^{10}	3.06922×10^{10}	1.55847×10^{13}	1.5683×10^{13}	9.63318×10^{15}	9.6445×10^{15}
5	3.42903×10^{10}	3.44143×10^{10}	1.8585×10^{13}	1.87265×10^{13}	1.22457×10^{16}	1.24349×10^{16}
6	3.76958×10^{10}	3.76835×10^{10}	2.14798×10^{13}	2.15861×10^{13}	1.4919×10^{16}	1.51619×10^{16}
7	4.08439×10^{10}	4.05663×10^{10}	2.42845×10^{13}	2.37201×10^{13}	1.76398×10^{16}	1.66972×10^{16}
8	4.37832×10^{10}	4.39075×10^{10}	2.70108×10^{13}	2.724×10^{13}	2.03988×10^{16}	2.06017×10^{16}
9	4.65486×10^{10}	4.65312×10^{10}	2.96679×10^{13}	2.94271×10^{13}	2.3189×10^{16}	2.26023×10^{16}
10	4.91663×10^{10}	4.91363×10^{10}	3.22631×10^{13}	3.24807×10^{13}	2.60051×10^{16}	2.69184×10^{16}
11	5.16565×10^{10}	5.17448×10^{10}	3.48022×10^{13}	3.47606×10^{13}	2.88433×10^{16}	2.87018×10^{16}
12	5.40352×10^{10}	5.39624×10^{10}	3.72905×10^{13}	3.73482×10^{13}	3.17002×10^{16}	3.18035×10^{16}
13	5.63152×10^{10}	5.65418×10^{10}	3.97319×10^{13}	4.00187×10^{13}	3.45733×10^{16}	3.48184×10^{16}
14	5.85072×10^{10}	5.83654×10^{10}	4.21303×10^{13}	4.1917×10^{13}	3.74603×10^{16}	3.70813×10^{16}
15	6.062×10^{10}	6.08708×10^{10}	4.44887×10^{13}	4.48257×10^{13}	4.03594×10^{16}	4.08236×10^{16}
16	6.2661×10^{10}	6.27652×10^{10}	4.68097×10^{13}	4.69566×10^{13}	4.32693×10^{16}	4.3287×10^{16}

Table 2
Conjecture vs. data for $k = 6, 7$, same intervals as the previous table

n	conj. $k=6$	data $k=6$	conj. $k=7$	data $k=7$
0	2.15456×10^{17}	2.08527×10^{17}	8.45652×10^{19}	7.99015×10^{19}
1	1.18835×10^{18}	1.20686×10^{18}	6.24627×10^{20}	6.3773×10^{20}
2	2.69034×10^{18}	2.66481×10^{18}	1.67709×10^{21}	1.66563×10^{21}
3	4.56155×10^{18}	4.56713×10^{18}	3.18661×10^{21}	3.25679×10^{21}
4	6.72399×10^{18}	6.61933×10^{18}	5.1125×10^{21}	4.87831×10^{21}
5	9.12928×10^{18}	9.3828×10^{18}	7.42365×10^{21}	7.74635×10^{21}
6	1.17439×10^{19}	1.21474×10^{19}	1.00952×10^{22}	1.06992×10^{22}
7	1.45431×10^{19}	1.31266×10^{19}	1.31065×10^{22}	1.11053×10^{22}
8	1.75076×10^{19}	1.75386×10^{19}	1.64403×10^{22}	1.61306×10^{22}
9	2.06221×10^{19}	1.95439×10^{19}	2.00815×10^{22}	1.83038×10^{22}
10	2.3874×10^{19}	2.61353×10^{19}	2.40171×10^{22}	2.8627×10^{22}
11	2.72527×10^{19}	2.70986×10^{19}	2.82354×10^{22}	2.82074×10^{22}
12	3.07492×10^{19}	3.06639×10^{19}	3.2726×10^{22}	3.20372×10^{22}
13	3.43557×10^{19}	3.43848×10^{19}	3.74797×10^{22}	3.70176×10^{22}
14	3.80656×10^{19}	3.7414×10^{19}	4.24878×10^{22}	4.13975×10^{22}
15	4.18729×10^{19}	4.25286×10^{19}	4.77427×10^{22}	4.86676×10^{22}
16	4.57724×10^{19}	4.53193×10^{19}	5.32373×10^{22}	5.1628×10^{22}
17	4.97592×10^{19}	4.98651×10^{19}	5.89648×10^{22}	6.0058×10^{22}

expansion for the $2k$th moment of ζ, so that taking more terms does not necessarily give an improvement. We therefore compared (5.1) to

$$\int_{100}^{D} \sum_{r=0}^{R} c_r(k) \log(t/2\pi)^{k^2-r}\, dt, \tag{5.3}$$

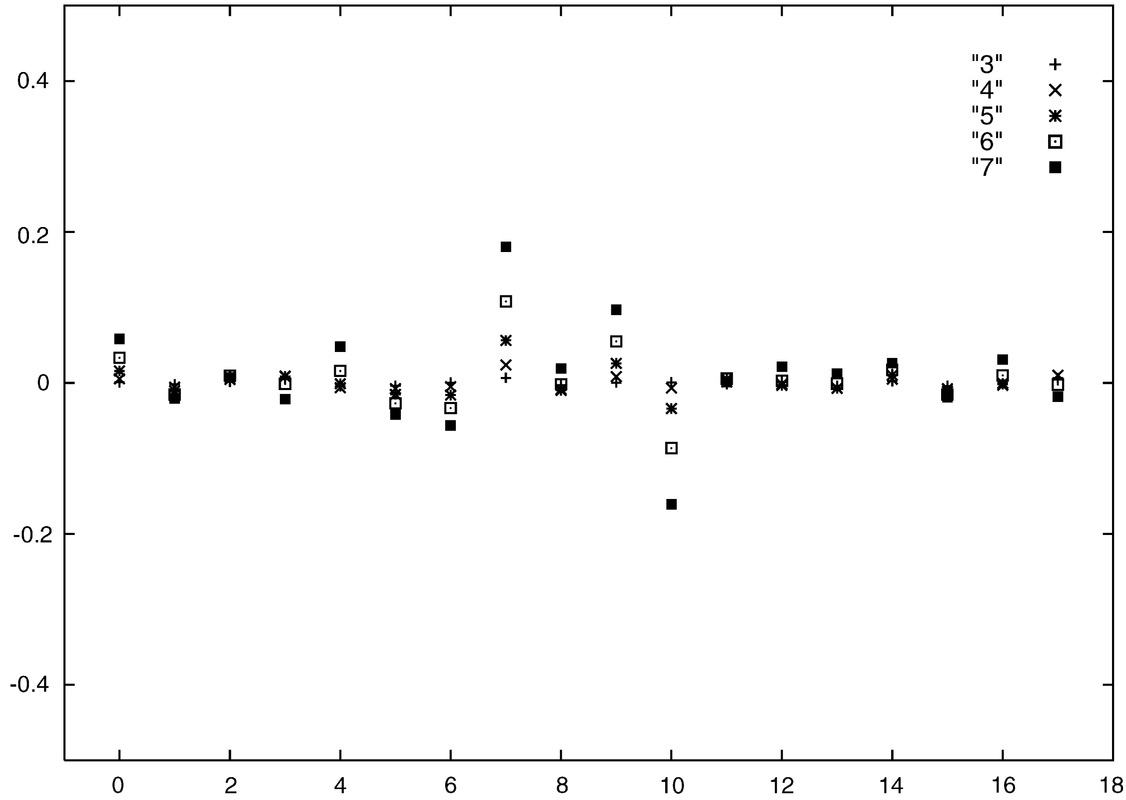

Fig. 1. The horizontal axis is n, and the vertical axis depicts (conjecture − data)/data for the values in Tables 1 and 2. For any finite interval, as $k \to \infty$, the main contribution to the $2k$th moment comes from the largest value of $|\zeta(1/2 + it)|^{2k}$ on that interval. This explains the feature that, for a fixed interval, the actual moment tends to progressively deviate from the conjectured value as k increases.

Table 3
The coefficients $c_R(k)$, and conjecture v.s. data for $k = 0.5$ for three intervals. The bottom row gives (5.1) for the interval $[100, D]$, with $D = 1000$, $10\,000$, and $100\,000$. For each D, we compare this to the value of (5.3), $R = 0, 1, \ldots, 7$

R	$c_R(0.5)$	(5.3), $D = 1000$	(5.3), $D = 10\,000$	(5.3), $D = 100\,000$
0	1.1299287453321533	1463.83	17768.4	193494
1	0.19628236755422853	1523.55	18258.1	197413
2	0.03248602185728907	1525.93	18271.4	197491
3	−0.5289095729314908	1516.37	18234.3	197335
4	3.2346669444094671	1531.24	18275.5	197459
5	−21.381296730027876	1505.43	18222.2	197343
6	166.38844209028643	1559.87	18310.8	197488
7	−1529.2695739774642	1419.97	18120.1	197237
(5.1)		1521.27	18257.1	197425

for a few values of D. We present our data in Tables 3–6, listing for each k, the values of $c_0(k), \ldots, c_7(k)$, and of (5.1) compared to (5.3) with $D = 1000, 10\,000$, and $100\,000$, and $R = 0, 1, \ldots, 7$.

While we have managed to explicitly determine the first few coefficients $c_r(k)$ of the moment polynomials $P_k(x)$, we have not yet managed to understand certain aspects of these polynomials,

Table 4
Conjecture vs. data for $k = 3.2$

R	$c_R(3.2)$	(5.3), $D = 1000$	(5.3), $D = 10\,000$	(5.3), $D = 100\,000$
0	$0.37531596173465401 \times 10^{-6}$	1968.83	1.16353×10^6	2.19960×10^8
1	$0.34462154217944847 \times 10^{-4}$	40049.5	1.65169×10^7	2.41753×10^9
2	$0.12662390083082525 \times 10^{-2}$	336190	9.78885×10^7	1.12289×10^{10}
3	$0.23963666452208821 \times 10^{-1}$	1.52891×10^6	3.2097×10^8	2.94868×10^{10}
4	0.2526426167678357	4.22213×10^6	6.6336×10^8	5.06417×10^{10}
5	1.5214668466274718	7.72205×10^6	9.6529×10^8	6.47041×10^{10}
6	5.3060442651520751	1.03793×10^7	1.12055×10^9	7.01449×10^{10}
7	11.121264784324178	1.16045×10^7	1.16894×10^9	7.14177×10^{10}
(5.1)		1.15305×10^7	1.16746×10^9	7.16886×10^{10}

Table 5
Conjecture vs. data for $k = 1.8$. For this value of k, and the range we examined, $R = 4$ or 5 give the best approximation

R	$c_R(1.8)$	(5.3), $D = 1000$	(5.3), $D = 10\,000$	(5.3), $D = 100\,000$
0	0.13885991555298723	15298.6	604203	1.58922×10^7
1	1.2590684761107478	46198.5	1.42746×10^6	3.20931×10^7
2	2.4174835075472416	59612.2	1.66821×10^6	3.56224×10^7
3	2.546894763686222	62863.9	1.70753×10^6	3.60492×10^7
4	−2.21426710514627	62199.9	1.7021×10^6	3.60059×10^7
5	3.223904454789757	62432.5	1.70339×10^6	3.60134×10^7
6	46.42674651960987	63260.1	1.70659×10^6	3.60268×10^7
7	−840.1304443557953	59448.3	1.69608×10^6	3.59953×10^7
(5.1)		61744.5	1.70134×10^6	3.60129×10^7

Table 6
Conjecture vs. data for $k = 0.5 + i$. The data here is not as convincing as for the other values of k, but, nonetheless, the early terms do give a reasonable approximation, and we believe the fit would improve with more substantial data

R	$c_R(0.5+i)$	(5.3), $D = 1000$	(5.3), $D = 10\,000$	(5.3), $D = 100\,000$
0	$1.3117481341987813 + 1.211708767666727i$	$-308.872 + 439.126i$	$-3698.00 + 2357.78i$	$-34129.1 + 8908.71i$
1	$-3.0693034820213132 + 2.309977688777579i$	$-508.454 + 246.589i$	$-4331.26 + 957.574i$	$-35042.9 - 44.9533i$
2	$23.861826126198446 - 5.4045694962616631i$	$-335.035 + 646.347i$	$-4243.1 + 2618.59i$	$-36981.1 + 6688.15i$
3	$-111.54278536885322 - 35.79807241977336i$	$-285.625 + 118.290i$	$-3667.307 + 1304.32i$	$-34054.1 + 3538.21i$
4	$828.16689710582718 + 437.514818042632i$	$-546.679 + 1199.98i$	$-4747.02 + 3257.57i$	$-37543.5 + 6786.35i$
5	$-5808.11341189128 - 8339.592888954564i$	$1514.537 - 1342.42i$	$-738.290 - 0.1097i$	$-30111.2 + 3451.52i$
6	$15613.29091863494 + 101218.4464636376i$	$-6736.01 + 2796.92i$	$-12358.2 + 3830.64i$	$-45377.2 + 5624.57i$
7	$188541.27977634034 - 1175857.723687032i$	$23708.43 - 2789.22i$	$24043.14 + 702.364i$	$-4932.63 + 6133.48i$
(5.1)		$-340.843 + 383.859i$	$-3946.25 + 1883.17i$	$-35140 + 4830.47i$

such as the uniform asymptotics of the coefficients, or uniform asymptotics of $P_k(x)$ with x a function of k. The latter is needed, for example, to properly understand how large $|\zeta(1/2 + it)|$ can get [FGH].

5.1. *Plots of* $c_r(k)$

We present in Figs. 2 and 3 some graphs of the coefficients $c_r(k)$ with $-1/2 < k < 11/2$, for $r = 0, 1, \dots, 7$.

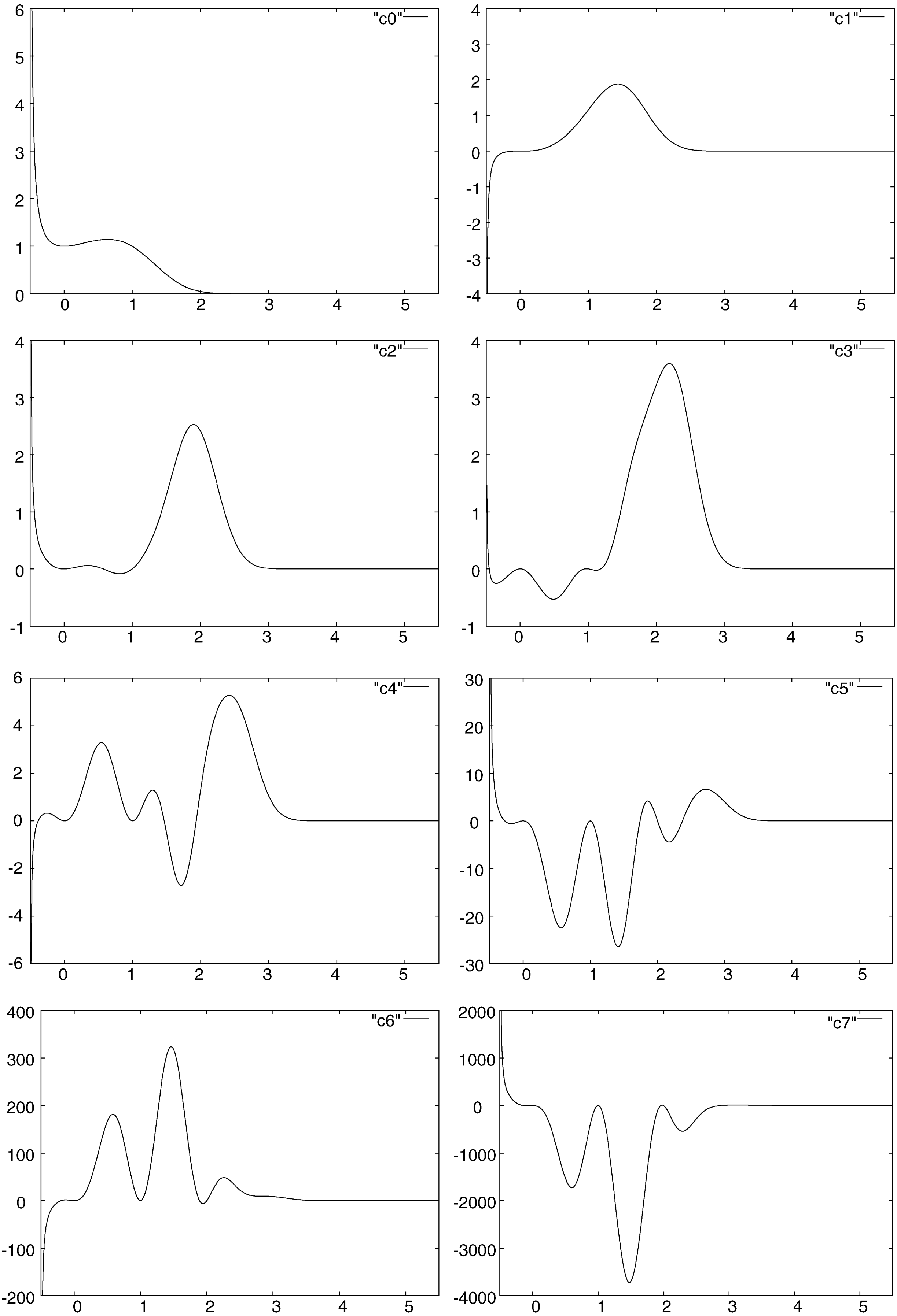

Fig. 2. Graphs of $c_r(k)$ with $-1/2 < k < 11/2$, for $r = 0, \ldots, 7$.

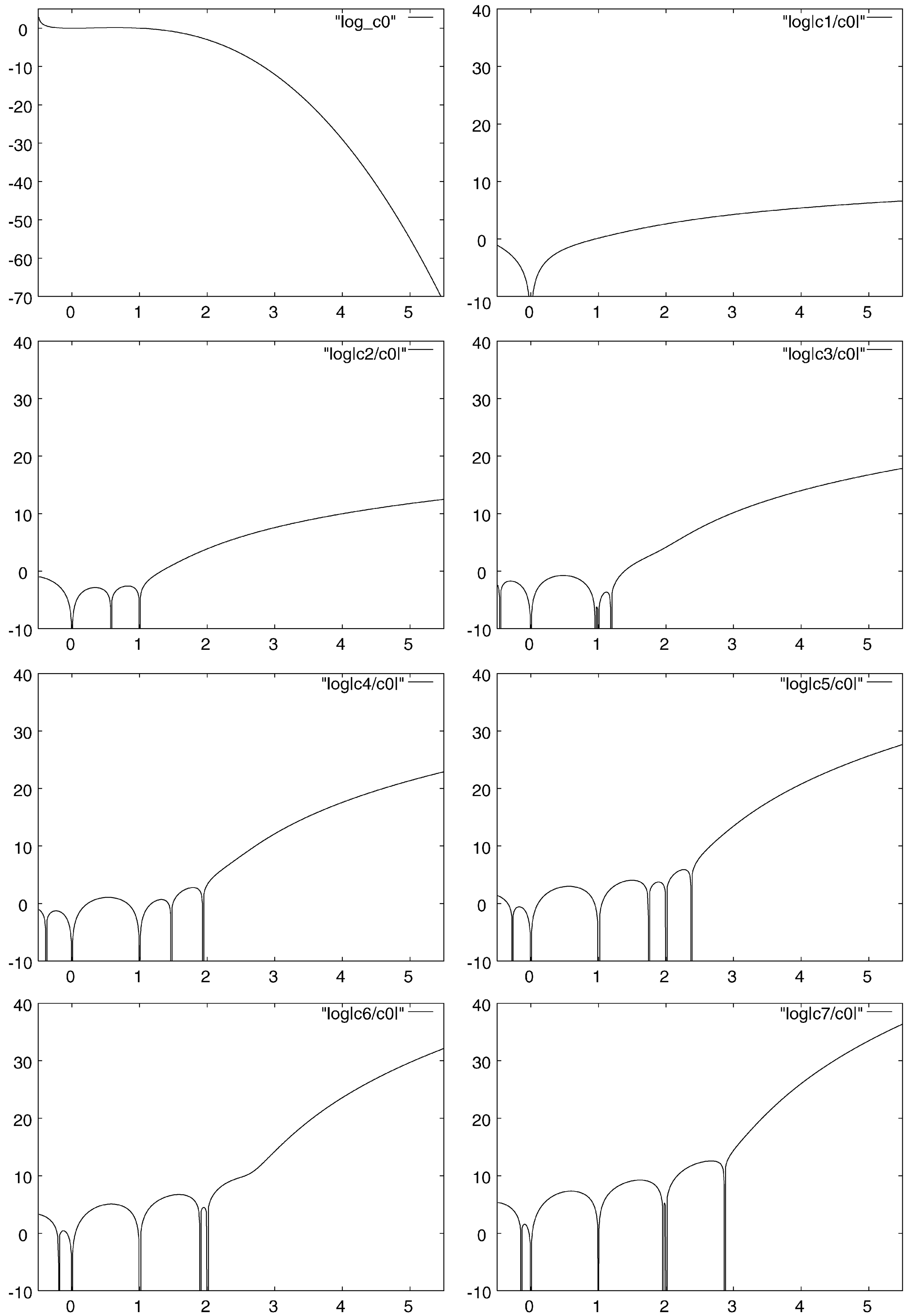

Fig. 3. The first figure depicts the graph of $\log(|c_0(k)|)$, while the next seven depict $\log(|c_r(k)/c_0(k)|)$, for $r = 1, \ldots, 7$. The asymptotic behavior of $\log(c_0(k))$ as $k \to \infty$ is implied by [CGo,KeS] and is, to leading order, $-k^2 \log(k)$. The cusps occur at zeros of $c_r(k)$, some of which are accounted for by the fact that, for non-negative $k \in \mathbb{Z}$, $P_k(x)$ is a polynomial of degree k^2 so that $c_r(k) = 0$ if $r > k^2$.

6. Remarks about other families: orthogonal and symplectic

In this paper we have explained two approaches for obtaining the coefficients $c_r(k)$ of $P_k(x)$. The first involves explicitly determining the residue on the r.h.s. of (1.2). Theorems 1.2–1.4, and the procedure given in Section 2 describe this in detail. The second approach involves using the combinatorial sum (1.11), using small shifts, and high precision.

The same methods can be taken for other families of L-functions, for instance in determining the lower order terms in the moments of $L(1/2, \chi_d)$, quadratic Dirichlet L-functions, or of $L_E(1/2, \chi_d)$, the L-functions associated to the quadratic twists of a given elliptic curve, to name just two examples, in both cases evaluated at the critical point. The former is an example of a unitary symplectic family, while the latter is an example of an orthogonal family [KaS]. See [CFKRS] where we discuss these examples in detail. As with the Riemann zeta function, conjectures are given for the full asymptotics of their moments, expressed in terms of multi-dimensional residues and also as combinatorial sums. In that paper, we used Method 2 of Section 4.2 for the analogous combinatorial sums to numerically compute lower terms for the moments, and verify the full asymptotics.

For the elliptic curve family, the next to leading term in the asymptotics of the moments has been worked out explicitly, and a test has been devised to verify the first two terms in the asymptotics of that particular family with an application to estimating the number of elliptic curves of rank greater than zero [CPRW]. See also [BMSW] for a survey of results related to the latter question.

Acknowledgments

J.B.C., D.W.F., and M.O.R. were supported by the NSF Focused Research Group grant DMS 0244660. J.P.K. was supported by an EPSRC Senior Research Fellowship. M.O.R. was also funded by NSERC. N.C.S. was supported by fellowships from the Royal Society and EPSRC. J.P.K., M.O.R., and N.C.S. wish to thank AIM for providing further support and an environment for collaborative work.

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