Advances in Mathematics 332 (2018) 311–348

Contents lists available at ScienceDirect

Advances in Mathematics

www.elsevier.com/locate/aim

Zeros of the deformed exponential function

Liuquan Wang [a], Cheng Zhang [b,*]

[a] School of Mathematics and Statistics, Wuhan University, Wuhan 430072, Hubei, People's Republic of China

[b] Department of Mathematics, Johns Hopkins University, Baltimore, MD 21218, United States

ARTICLE INFO

Article history:
Received 7 January 2018
Received in revised form 4 April 2018
Accepted 20 April 2018
Available online 26 May 2018
Communicated by George Andrews

MSC:
primary 30C15, 11B83, 41A60
secondary 11M36, 34K06

Keywords:
Deformed exponential function
Asymptotic expansion
Eisenstein series
Bernoulli numbers

ABSTRACT

Let $f(x)=\sum_{n=0}^{\infty}\frac{1}{n!}q^{n(n-1)/2}x^n$ $(0<q<1)$ be the deformed exponential function. It is known that the zeros of $f(x)$ are real and form a negative decreasing sequence (x_k) $(k\geq 1)$. We investigate the complete asymptotic expansion for x_k and prove that for any $n\geq 1$, as $k\to\infty$,

$$x_k=-kq^{1-k}\Big(1+\sum_{i=1}^{n}C_i(q)k^{-1-i}+o(k^{-1-n})\Big),$$

where $C_i(q)$ are some q series which can be determined recursively. We show that each $C_i(q)\in\mathbb{Q}[A_0,A_1,A_2]$, where $A_i=\sum_{m=1}^{\infty}m^i\sigma(m)q^m$ and $\sigma(m)$ denotes the sum of positive divisors of m. When writing C_i as a polynomial in A_0, A_1 and A_2, we find explicit formulas for the coefficients of the linear terms by using Bernoulli numbers. Moreover, we also prove that $C_i(q)\in\mathbb{Q}[E_2,E_4,E_6]$, where E_2, E_4 and E_6 are the classical Eisenstein series of weight 2, 4 and 6, respectively.

* Corresponding author.
E-mail addresses: wanglq@whu.edu.cn, mathlqwang@163.com (L. Wang), czhang67@jhu.edu (C. Zhang).

https://doi.org/10.1016/j.aim.2018.05.006

1. Introduction

Consider the function

$$f(x) := \sum_{n=0}^{\infty} \frac{x^n}{n!} q^{n(n-1)/2} \tag{1.1}$$

where $x, q \in \mathbb{C},\ |q| \leq 1$. The function $f(x)$ is entire and is called the "deformed exponential function" since it reduces to $\exp(x)$ when $q = 1$. It appears naturally and frequently in pure and applied mathematics. In combinatorics, the function $f(x)$ relates closely to the generating function for Tutte polynomials of the complete graph K_n [24], the enumeration of acyclic digraphs [18] and inversions of trees [15]. It also relates to the Whittaker and Goncharov constants [2] in complex analysis, and the partition function of one-site lattice gas with fugacity x and two-particle Boltzmann weight q in statistical mechanics [19]. Moreover, one can verify that this function is the unique solution to the functional differential equation

$$y'(x) = y(qx),\ y(0) = 1, \tag{1.2}$$

which is a special case of the "pantograph equation" [6]. For more detailed discussions on this function, we may refer to the notes from Alan Sokal's talks [20].

Surprisingly, many important properties of this function remain open, e.g., the distribution of its zeros. In 1952, Nassif [17] studied (on Littlewood's suggestion) the asymptotic behaviours and the zeros of the entire function

$$\sum_{n=0}^{\infty} e^{n^2\sqrt{2}\pi i} z^{2n}/n!,$$

which equals to $f(q^{\frac{1}{2}} z^2)$ with $q = e^{2\sqrt{2}\pi i}$. He used the fact that $\sqrt{2}$ has a periodic continued fraction expansion. Later, Littlewood [11,12] considered generalizations to Taylor series whose coefficients have smoothly varying moduli and arguments of the form $e^{n^2 \alpha\pi i}$, where α is a quadratic irrationality. See also [4,10,13,23] for the studies on the behaviours of these functions. To our knowledge, for general complex number q satisfying $|q| \leq 1$, the distribution of the zeros of $f(x)$ has not been completely understood up to now. A theorem of Eremenko cited in [21] considered the case where q lies in any compact set of the open unit disk $\mathbb{D}$. There are relatively more works on the model case where $0 < q < 1$. In 1972, Morris et al. [5] used a theorem of Laguerre to show that $f(x)$ has infinitely many real zeros and these zeros are all negative and simple. They also proved that there is no other zero for the analytic extension (to the complex plane) of $f(x)$ by using the so-called multiplier sequence (a modest gap in their proof was filled by Iserles [8]). Therefore, when $0 < q < 1$, the zeros of $f(x)$ form one strictly decreasing sequence of negative numbers (x_k) $(k \geq 1)$. We remark that in some previous works (e.g., [9,22]), the subscripts of the sequence start with 0 rather than 1. In this paper, as well as in [25], the subscripts start with 1 for the elegance of notation.

When $0 < q < 1$, some conjectures on the zeros x_k ($k \geq 1$) have been proposed in [5,8,18]. For example, Morris et al. [5] conjectured that

$$\lim_{k\to\infty} \frac{x_{k+1}}{x_k} = \frac{1}{q}. \tag{1.3}$$

In 1973, Robinson [18] also derived (1.2) when counting the labeled acyclic digraphs. He speculated that

$$x_k = -kq^{1-k} + o(q^{1-k}). \tag{1.4}$$

These conjectures have been investigated by several authors (see e.g., [7,9,14,22]). In particular, Langley [9] showed that as $k \to \infty$

$$\frac{x_{k+1}}{x_k} = \frac{1}{q}\Big(1 + \frac{1}{k}\Big) + o(k^{-2}). \tag{1.5}$$

He also proved that there exists a positive constant γ, which is independent of k, such that

$$x_k = -kq^{1-k}(\gamma + o(1)). \tag{1.6}$$

As a consequence, (1.3) is true. Recently, one of the authors [25] refined Langley's work and confirmed the observation (1.4). Indeed, he showed that as $k \to \infty$,

$$x_k = -kq^{1-k}\Big(1 + \sum_{m=1}^{\infty} \sigma(m) q^m k^{-2} + o(k^{-2})\Big). \tag{1.7}$$

Here for any positive integer n,

$$\sigma(n) := \sum_{d|n,\ d>0} d.$$

Later Derfel et al. [3] studied the asymptotic behaviours of the zeros of solutions of (1.2) with different initial conditions instead of the restriction $y(0) = 1$.

Our research on the zeros of the deformed exponential function is motivated by the conjectures introduced by Sokal [21] in his talk at Institut Henri Poincaré in 2009. In this paper, we obtain a complete asymptotic expansion formula for the zeros x_k when $0 < q < 1$. To be more specific, we will approximate x_k with remainder term $o(k^{-n-1})$ for any $n \geq 1$. We also establish the connection between the classical Eisenstein series and the zeros of the deformed exponential function. To state our results, we define for $i \geq 0$,

$$A_i = A_i(q) := \sum_{m=1}^{\infty} m^i \sigma(m) q^m. \tag{1.8}$$

Theorem 1. *Let $0 < q < 1$ and $n \geq 1$. Then as $k \to \infty$,*

$$x_k = -kq^{1-k}\Big(1 + \sum_{i=1}^{n} C_i(q) k^{-1-i} + o(k^{-1-n})\Big), \tag{1.9}$$

where each $C_i(q)$ is a multivariate polynomial in $A_0, A_1, ..., A_{i-1}$ with rational coefficients. These polynomials can be determined recursively.

Remark 1. For example, $C_1 = A_0$, $C_2 = -A_1$, $C_3 = -\frac{1}{10}A_0 + \frac{3}{5}A_1 + \frac{1}{2}A_2 - \frac{13}{10}A_0^2$. The recurrence relation and the basic structure of these polynomials will be presented in Sections 3 and 4. Moreover, we conjecture that (1.9) should hold for any complex number q satisfying $0 < |q| < 1$ (and even for some q satisfying $|q| = 1$), if the complex zeros are listed according to their multiplicities and ordered by increasing modulus. Furthermore, it is interesting to consider if one could obtain similar results for the zeros of the rescaled Rogers–Ramanujan function [22]

$$\tilde{R}(x; y, q) = \sum_{n=0}^{\infty} \frac{x^n q^{n(n-1)/2}}{(1+y)(1+y+y^2)\cdots(1+y+\cdots+y^{n-1})},$$

which reduces to a “partial theta function” when $y = 0$, and the “deformed exponential function” when $y = 1$.

When $n \geq 4$, we observe that the expression of $C_n(q)$ in terms of $A_0, A_1, \ldots, A_{n-1}$ is not unique. The polynomial given by the recurrence relation in Theorem 1 is just one candidate. For example, we have

$$\begin{aligned} C_4 &= \frac{1}{10}A_1 - \frac{14}{15}A_2 - \frac{1}{6}A_3 + \frac{23}{5}A_0A_1 \\ &= \frac{1}{10}A_1 - \frac{11}{10}A_2 + \frac{23}{5}A_0A_1 - 6A_1^2 + 4A_0A_2. \end{aligned} \tag{1.10}$$

Thus we continue to study the relations between A_i’s. Indeed, the following identity is established

$$A_3 = A_2 + 36A_1^2 - 24A_0A_2.$$

Differentiating it with respect to q gives more similar identities on A_i’s. Therefore, we find that it is possible to express C_n as a polynomial in just A_0, A_1 and A_2. Furthermore, the coefficients of the linear terms in that polynomial can be given explicitly using Bernoulli numbers. Let B_n be the n-th Bernoulli number. It is well known that $B_{2m+1} = 0$ for all $m \geq 1$. The first few values of B_i are $B_0 = 1$, $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$ and $B_4 = -\frac{1}{30}$.

Theorem 2. *For any $n \geq 1$, C_n can be expressed as a trivariate polynomial in A_0, A_1 and A_2 with rational coefficients. This polynomial is unique and for $n \geq 2$, we have*

$$C_{2n-1} = \frac{6B_{2n}}{n} A_0 - \frac{36B_{2n}}{n} A_1 + \left(1 + \frac{30B_{2n}}{n}\right) A_2 + \text{higher degree terms},$$
$$C_{2n} = -\frac{6B_{2n}}{n} A_1 + \left(\frac{6B_{2n}}{n} - 1\right) A_2 + \text{higher degree terms}.$$

Remark 2. For example, we find that

$$\begin{aligned} C_5 =& \frac{1}{21} A_0 - \frac{2}{7} A_1 + \frac{26}{21} A_2 + \frac{53}{70} A_0^2 + 22 A_1^2 - 36 A_0 A_1^2 \\ & - \frac{159}{35} A_0 A_1 - \frac{43}{2} A_0 A_2 + 2 A_1 A_2 + \frac{737}{210} A_0^3 + 24 A_0^2 A_2, \\ C_6 =& -\frac{1}{21} A_1 - \frac{20}{21} A_2 - \frac{74}{35} A_0 A_1 - \frac{1401}{35} A_1^2 - \frac{2}{5} A_2^2 + \frac{705}{14} A_0 A_2 \\ & - \frac{101}{10} A_1 A_2 + \frac{1662}{5} A_0 A_1^2 - \frac{321}{14} A_0^2 A_1 - \frac{36}{5} A_1^3 \\ & - \frac{1132}{5} A_0^2 A_2 - \frac{864}{5} A_0^2 A_1^2 + \frac{72}{5} A_0 A_1 A_2 + \frac{576}{5} A_0^3 A_2. \end{aligned}$$

The Bernoulli numbers in the linear terms are from Faulhaber's formula for the power sum of the first m positive integers (see (2.49)). As shown in the examples above, the higher degree terms look much more complicated than the linear terms, though they can be explicitly derived from the recurrence relation of C_n (see (4.1)), which is essentially determined by the expressions of the unsigned Stirling numbers of the first kind (see (2.24), (2.46)).

Let

$$E_2 = E_2(q) := 1 - 24 \sum_{n=1}^{\infty} \frac{nq^n}{1-q^n}, \tag{1.11}$$

$$E_4 = E_4(q) := 1 + 240 \sum_{n=1}^{\infty} \frac{n^3 q^n}{1-q^n}, \tag{1.12}$$

$$E_6 = E_6(q) := 1 - 504 \sum_{n=1}^{\infty} \frac{n^5 q^n}{1-q^n}. \tag{1.13}$$

It is well known that E_2, E_4 and E_6 are classical Eisenstein series on the full modular group

$$SL(2, \mathbb{Z}) = \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mid ad - bc = 1,\ a, b, c, d \in \mathbb{Z} \right\}.$$

We will show that A_0, A_1 and A_2 can be represented as polynomials in E_2, E_4 and E_6 with rational coefficients and vice versa. Namely,

$$\mathbb{Q}[A_0, A_1, A_2] = \mathbb{Q}[E_2, E_4, E_6].$$

Since it is well known that E_2, E_4 and E_6 are algebraically independent over $\mathbb{C}$ (see e.g., [16, Lemma 117]), it follows that A_0, A_1 and A_2 are also algebraically independent over $\mathbb{C}$. So Theorem 2 implies that $C_n(q)$ are in the ring of quasimodular forms on $SL(2,\mathbb{Z})$.

Corollary 1. *Let $n \geq 1$. Then $C_n(q) \in \mathbb{Q}[E_2, E_4, E_6]$.*

The paper is organized as follows. In Section 2, we study the series expansion of $f(-(k + ak^{-1})q^{1-k})$ for large k, where $a = a(k^{-1})$ is positive and bounded for large k. Here one can think of $-(k+ak^{-1})q^{1-k}$ as a "prospective root" of f. We observe that the first $2k$ terms of this series dominate the others, so these $2k$ terms are carefully analyzed in Lemmas 1 and 2. Most of these terms enjoy nice properties described in Lemma 1, while others are more subtle and related to the series expansion of (2.17). Lemma 2 gives the formula of the coefficient of each term in the series expansion of (2.17). In the proof of Lemma 2, the properties of elementary symmetric polynomials and complete homogeneous symmetric polynomials play an important role.

In Section 3, we prove Theorem 1. We first define C_n recursively (see (3.3)) by exploiting the coefficients of the series expansion of (2.17). Let $a = \sum_{i=1}^{n-1} C_i k^{-(i-1)} + \lambda k^{-(n-1)}$. Then we use Lemmas 1 and 2 to show that if $\lambda \neq C_n$, and in addition that $\lambda > 0$ when $n = 1$, then

$$(-1)^k(\lambda - C_n) f(-(k + ak^{-1})q^{1-k}) > 0.$$

This allows us to determine the signs of $f(x)$ at the endpoints of certain intervals. We finish the proof of Theorem 1 by the intermediate value theorem and (1.5).

In Section 4, we study various representations of C_n. In Section 4.1, we give more details on the recursive formula of C_n, and prove that C_n can be written as a multivariate polynomial of $A_0, A_1, \ldots, A_{n-1}$, in which the coefficient of A_{n-1} is $\frac{(-1)^{n-1}}{(n-1)!}$ (Proposition 5). In Section 4.2, we continue to discuss the structure of the multivariate polynomial representation of C_n by those A_i's, especially the linear terms. In particular, we show in Proposition 6 that the sum of the coefficients of the linear terms $A_0, A_1, \ldots, A_{n-1}$ in C_n equals to $(-1)^{n-1}$. Furthermore, we give explicit formulas for the coefficients of the linear terms A_0 and A_1 in Propositions 7 and 8. In Section 4.3, we first establish the relations between the classical Eisenstein series and our A_i's (Proposition 9). Then we show in Lemma 10 that each A_n can be written as a multivariate polynomial in A_0, A_1 and A_2. Combining these facts, we complete the proof of Theorem 2.

Remark 3. It may be illuminating to consider (1.9) as a formal power series. Suppose that $C_i(q) = \sum_{j=1}^{\infty} C_{ij} q^j$. Using formal power series, we denote $F_j(t) := \sum_{i=1}^{\infty} C_{ij} t^{i+1}$. Then one may rewrite (1.9) as a formal power series

$$x_k(q) \sim -kq^{1-k}\Big(1 + \sum_{j=1}^{\infty} F_j(k^{-1})q^j\Big). \tag{1.14}$$

We observe that the formal power series (1.14) numerically agrees with the expansion in q of the k-th zero given in [21, p. 14]. (Note that in [21] the sequence (x_k) starts with subscript 0 and for each j, $F_j(k^{-1})$ is a rational function in k.) It was conjectured by Sokal [21, p. 11] that

$$F_j(k^{-1}) \geq 0$$

for all integers $j, k \geq 1$. This conjecture is still open, even for fixed $k = 1$. In particular, we will see that $C_{i1} = (-1)^{i+1}$ by Proposition 6, which implies that

$$F_1(k^{-1}) = \frac{1}{k(k+1)}.$$

This verifies the case $j = 1$. For $j \geq 2$, we find that the difficulty to obtain the closed form of $F_j(k^{-1})$ lies in the complexity of the higher degree terms in Theorem 2.

2. Preliminary results

Throughout this paper, we fix q with $0 < q < 1$. We use the notation "$O(k^{-m})$" to denote the class of functions of k which is bounded by Ck^{-m}, where C is a constant that is dependent on the fixed parameters but independent of k. Let $a = a(k^{-1})$ be a function in k satisfying that $a = a_0 + O(k^{-1})$ where $a_0 > 0$ is a constant. The main goal of this section is to study the values of $f(-(k + ak^{-1})q^{1-k})$ for large k.

We first observe that

$$f(-(k + ak^{-1})q^{1-k}) = \sum_{n=0}^{\infty} (-1)^n u_n, \tag{2.1}$$

where

$$u_n = \frac{(k + ak^{-1})^n}{n!} q^{-n(2k-n-1)/2}.$$

In order to prove Theorem 1, we will select some special functions as a (see Section 3). For these a and sufficiently large k, we will see that for the sum in (2.1), the first $2k$ terms dominate the others. Therefore, we rewrite (2.1) as

$$f(-(k+ak^{-1})q^{1-k}) = \sum_{n=0}^{2k-1}(-1)^n u_n + \sum_{n=2k}^{\infty}(-1)^n u_n = \sum_{j=0}^{k-1}(-1)^{j-1}v_j + \sum_{n=2k}^{\infty}(-1)^n u_n, \tag{2.2}$$

where we denote

$$v_j = u_{2k-j-1} - u_j \quad (0 \le j \le k-1).$$

The following lemma shows the positivity and "almost monotonicity" of the sequence v_j.

Lemma 1. *There exists a positive integer $K(q)$ such that for any $k \ge K(q)$,*

$$v_j > 0, \qquad 0 \le j \le k-1.$$

Furthermore, there exists a positive integer $N(q)$ such that for any $N \ge N(q)$ and $k \ge q^{-3N}$,

$$v_j < v_{j+1}, \qquad 0 \le j \le k-N.$$

Proof. Since $a = a_0 + O(k^{-1})$ and $a_0 > 0$, we can find a positive integer $K(q)$ such that $a > 0$ for any $k \ge K(q)$. Now we assume that $k \ge K(q)$. By the AM-GM inequality, we have

$$\begin{aligned}\prod_{i=1}^{2k-1-2j}(j+i) &< \left(\frac{\sum_{i=1}^{2k-1-2j}(j+i)}{2k-1-2j}\right)^{2k-1-2j} \\ &= k^{2k-1-2j} \\ &< (k+ak^{-1})^{2k-1-2j} \quad (0 \le j \le k-1).\end{aligned} \tag{2.3}$$

This implies

$$\frac{(k+ak^{-1})^j}{j!} < \frac{(k+ak^{-1})^{2k-1-j}}{(2k-1-j)!} \quad (0 \le j \le k-1).$$

So

$$u_j < u_{2k-1-j} \quad (0 \le j \le k-1),$$

which gives the first inequality.

Note that

$$v_{j+1} = q^{(j+1)(j+2-2k)/2}\frac{(k+ak^{-1})^{2k-j-2}}{(2k-2-j)!}(1-w_j) \tag{2.4}$$

where

$$w_j = \frac{(2k-2-j)!}{(j+1)!(k+ak^{-1})^{2k-3-2j}}.$$

Since we have proved that $v_{j+1} > 0$, it follows that

$$0 < w_j < 1$$

By the AM-GM inequality,

$$\frac{w_{j+1}}{w_j} = \frac{(k+ak^{-1})^2}{(j+2)(2k-2-j)} > 1.$$

By (2.4), we see that $v_j < v_{j+1}$ is equivalent to

$$q^{j+1-k}(1-w_j) > \frac{k+ak^{-1}}{2k-j-1}(1-w_{j-1}). \tag{2.5}$$

Using the relation

$$w_{j-1} = \frac{(j+1)(2k-j-1)}{(k+ak^{-1})^2} w_j,$$

we see that (2.5) is equivalent to

$$\left(q^{-k+j+1} - \frac{j+1}{k+ak^{-1}}\right) w_j < q^{-k+j+1} - \frac{k+ak^{-1}}{2k-1-j}. \tag{2.6}$$

For some positive integer N, we denote

$$t = 2k-1-j \quad (k+N-1 \le t \le 2k-1)$$

and

$$g(t) = \frac{1}{t} - \frac{(2k-t)w_{k-N}}{(k+ak^{-1})^2} - q^{k-t}\left(\frac{1-w_{k-N}}{k+ak^{-1}}\right).$$

Direct calculation yields

$$g'(t) = -\frac{1}{t^2} + \frac{w_{k-N}}{(k+ak^{-1})^2} + \left(\frac{1-w_{k-N}}{k+ak^{-1}}\right) q^{k-t} \ln q \tag{2.7}$$

and

$$g''(t) = \frac{2}{t^3} - \left(\frac{1-w_{k-N}}{k+ak^{-1}}\right) q^{k-t} (\ln q)^2. \tag{2.8}$$

Since $0 < w_j < 1$, $g''(t)$ is decreasing for $t > 0$.

Note that when N is large enough ($N \geq N_1(q)$), we have $k \geq q^{-3N} \geq \max\{K(q), N^6\}$. Hence

$$\begin{aligned}\frac{1}{k+N-1} &= k^{-1}\left(1-(N-1)k^{-1}+(N-1)^2k^{-2}+O(N^3k^{-3})\right)\\ &= k^{-1}-(N-1)k^{-2}+(N-1)^2k^{-3}+O(k^{-7/2}). \end{aligned} \tag{2.9}$$

Similarly we have

$$\frac{1}{(k+N-1)^2} = k^{-2}-2(N-1)k^{-3}+O(k^{-11/3}) \tag{2.10}$$

and

$$\frac{1}{(k+N-1)^3} = k^{-3}+O(k^{-23/6}). \tag{2.11}$$

Next,

$$\begin{aligned} w_{k-N} &= \prod_{t=-N+2}^{N-2} \frac{k+t}{k+ak^{-1}}\\ &= \prod_{t=-N+2}^{N-2}\left(1+\frac{t}{k}\right)\left(1-\frac{a_0}{k^2}+O(k^{-3})\right)\\ &= \prod_{t=-N+2}^{N-2}\left(1+\frac{t}{k}-\frac{a_0}{k^2}-\frac{a_0t}{k^3}+O(k^{-3})\right)\\ &= 1-a_0(2N-3)k^{-2}+\sum_{-N+2\leq t_1<t_2\leq N-2}\frac{t_1t_2}{k^2}+O(k^{-17/6})\\ &= 1-a_0(2N-3)k^{-2}-\frac{(N-2)(N-1)(2N-3)}{6}k^{-2}+O(k^{-17/6}). \end{aligned}$$

Hence

$$\begin{aligned} \frac{1-w_{k-N}}{k+ak^{-1}} =& \frac{1}{k}\left(1-a_0k^{-2}+O(k^{-3})\right)\\ &\cdot\left(a_0(2N-3)k^{-2}+\frac{(N-2)(N-1)(2N-3)}{6}k^{-2}+O(k^{-17/6})\right)\\ =& \left(a_0(2N-3)+\frac{(N-2)(N-1)(2N-3)}{6}\right)k^{-3}+O(k^{-23/6}). \end{aligned} \tag{2.12}$$

Note that $k \geq q^{-3N}$ implies $q^{-N} = O(k^{1/3})$. Now by (2.11) and (2.12), we deduce that

$$g''(k+N-1) = \left(2 - c_N q^{1-N}(\ln q)^2\right) k^{-3} + O(k^{-7/2})$$

where

$$c_N := a_0(2N-3) + \frac{1}{6}(N-2)(N-1)(2N-3).$$

Similarly, we have

$$g'(k+N-1) = \left(2N-2 + c_N q^{1-N}\ln q\right) k^{-3} + O(k^{-7/2}).$$

When N is sufficiently large ($N \geq N_2(q) \geq N_1(q)$), we will have

$$g''(k+N-1) < 0,$$

and

$$g'(k+N-1) < 0.$$

So $g'(t)$ and $g(t)$ are also decreasing for $t \geq k+N-1$.

In the same way, we find that

$$g(k+N-1) = \left(a_0(2N-1) + \frac{N}{6}(N-1)(2N-1) - c_N q^{1-N}\right) k^{-3} + O(k^{-10/3}).$$

When N is large enough ($N \geq N(q) \geq N_2(q)$), we have

$$g(k+N-1) < 0.$$

So if $N \geq N(q)$ and $k \geq q^{-3N}$, we have

$$g(t) \leq g(k+N-1) < 0, \quad t \geq k+N-1.$$

Therefore,

$$\frac{1}{2k-1-j} - \frac{(j+1)w_{k-N}}{(k+ak^{-1})^2} - q^{-k+j+1}\left(\frac{1-w_{k-N}}{k+ak^{-1}}\right) < 0 \quad (0 \leq j \leq k-N).$$

This implies

$$\left(q^{-k+j+1} - \frac{j+1}{k+ak^{-1}}\right) w_{k-N} < q^{-k+j+1} - \frac{k+ak^{-1}}{2k-1-j} \quad (0 \leq j \leq k-N).$$

Since $w_j < w_{j+1}$, we have

$$\left(q^{-k+j+1} - \frac{j+1}{k+ak^{-1}}\right) w_j < q^{-k+j+1} - \frac{k+ak^{-1}}{2k-1-j} \quad (0 \leq j \leq k-N).$$

This proves (2.6) and hence the fact that

$$v_j < v_{j+1} \quad (0 \le j \le k-N). \quad \square$$

However, the sequence v_j may not be monotone when $k-N < j \le k-1$. So we need more delicate analysis on these v_j's, which is the crux of the problem. For $1 \le j \le N$,

$$\begin{aligned} v_{k-j} = u_{k+j-1} - u_{k-j} &= \Big(\frac{(k+ak^{-1})^{k+j-1}}{(k+j-1)!} - \frac{(k+ak^{-1})^{k-j}}{(k-j)!}\Big) q^{-(k+j-1)(k-j)/2} \\ &= \left(\prod_{i=1}^{j-1} \frac{k+ak^{-1}}{k+i} - \prod_{i=1-j}^{0} \frac{k+i}{k+ak^{-1}}\right) (k+ak^{-1})^k \frac{1}{k!} q^{-(k+j-1)(k-j)/2} \\ &= \left(\prod_{i=0}^{j-1} \frac{1+ak^{-2}}{1+ik^{-1}} - \prod_{i=1-j}^{-1} \frac{1+ik^{-1}}{1+ak^{-2}}\right) \frac{1+ak^{-2}}{k^{-2}} \\ &\quad \cdot q^{j(j-1)/2} \cdot (k+ak^{-1})^{k-2} \frac{1}{k!} q^{-k(k-1)/2}. \end{aligned} \tag{2.13}$$

We define for $j \ge 1$,

$$G(\alpha; x) := \prod_{i=0}^{j-1} \frac{1+\alpha x^2}{1+ix}, \tag{2.14}$$

$$H(\alpha; x) := \prod_{i=1-j}^{-1} \frac{1+ix}{1+\alpha x^2}. \tag{2.15}$$

In particular, when $j = 1$ we have $G(\alpha; x) = 1 + \alpha x^2$ and $H(\alpha; x) = 1$ since we agree that the empty product equals 1. It is then clear from (2.13) that

$$v_{k-j} = \big(G(a; k^{-1}) - H(a; k^{-1})\big) \frac{1+ak^{-2}}{k^{-2}} \cdot q^{j(j-1)/2} \cdot (k+ak^{-1})^{k-2} \frac{1}{k!} q^{-k(k-1)/2}. \tag{2.16}$$

Now we analyze the series expansion of the product

$$\frac{G(\alpha; x) - H(\alpha; x)}{x^2} \big(1 + \alpha x^2\big) \tag{2.17}$$

for α being a power series of x.

Lemma 2. *Let*

$$\alpha(x) := \sum_{i=0}^{\infty} a_i x^i. \tag{2.18}$$

For $n \geq 1$, the coefficient of x^{n-1} in the expansion of

$$\frac{G(\alpha(x);x) - H(\alpha(x);x)}{x^2}(1 + \alpha(x)x^2)$$

has the form

$$\mu(a_{n-1} + S_0(n) + S_1(n)\nu + S_2(n)\nu^2 + ... + S_n(n)\nu^n), \tag{2.19}$$

where $\mu = 2j - 1$, $\nu = j(j-1)$, and each $S_i(n)$ is a polynomial of $a_0, a_1, ..., a_{n-2}$, which is independent of j and has rational coefficients. In particular, $S_0(1) = S_0(2) = 0$ and $S_1(1) = \frac{1}{6}$.

The rest of this section will be devoted to giving a proof of Lemma 2. First, we compute the coefficients in the expansions $G(\alpha;x)$ and $H(\alpha;x)$ as power series in x regarding α as a parameter. That is,

$$G(\alpha;x) = \sum_{N=0}^{\infty} G_N x^N, \quad H(\alpha;x) = \sum_{N=0}^{\infty} H_N x^N,$$

where G_N and H_N are polynomials of α with coefficients depending on j. For example,

$$\begin{aligned}
G_0 =& H_0 = 1, \\
G_1 =& H_1 = -\tfrac{1}{2}j(j-1), \\
G_2 =& \tfrac{1}{24}(j-1)j(j+1)(3j-2) + j\alpha, \\
H_2 =& \tfrac{1}{24}(j-2)(j-1)j(3j-1) + (1-j)\alpha, \\
G_3 =& -\tfrac{1}{48}(j-1)^2j^2(j+1)(j+2) - \tfrac{1}{2}(j-1)j^2\alpha, \\
H_3 =& -\tfrac{1}{48}(j-3)(j-2)(j-1)^2j^2 + \tfrac{1}{2}(j-1)^2j\alpha.
\end{aligned}$$

To represent G_N and H_N, we define for $j \geq 1$ and $i \geq 0$ that

$$q_i(j) := e_i(1, 2, \cdots, j-1), \tag{2.20}$$

$$Q_i(j) := (-1)^i h_i(1, 2, \cdots, j-1) \tag{2.21}$$

where

$$e_i(X_1, X_2, \cdots, X_n) = \sum_{1 \leq n_1 < n_2 < \cdots < n_i \leq n} X_{n_1} X_{n_2} \cdots X_{n_i} \tag{2.22}$$

and

$$h_i(X_1, X_2, \cdots, X_n) = \sum_{1 \leq n_1 \leq n_2 \leq \cdots \leq n_i \leq n} X_{n_1} X_{n_2} \cdots X_{n_i} \tag{2.23}$$

are elementary symmetric polynomials and complete homogeneous symmetric polynomials respectively. Note that here we agree that

$$e_0(X_1, X_2, \cdots, X_n) = h_0(X_1, X_2, \cdots, X_n) = 1$$

so that $q_0(j) = Q_0(j) = 1$. By definition it is clear that $q_i(j) = Q_i(j) = 0$ if $i \geq j$. Moreover, we remark that $q_i(j)$ is just the unsigned Stirling numbers of the first kind

$$q_i(j) = c(j, j - i). \tag{2.24}$$

It is not difficult to see that

$$\sum_{k=0}^{\infty} e_k(X_1, X_2, \cdots, X_n)t^k = \prod_{i=1}^{n}(1 + X_i t), \tag{2.25}$$

$$\sum_{k=0}^{\infty} h_k(X_1, X_2, \cdots, X_n)t^k = \prod_{i=1}^{n} \frac{1}{1 - X_i t}. \tag{2.26}$$

These identities imply the following well-known fundamental relation: for $m \geq 1$,

$$\sum_{i=0}^{m}(-1)^i e_i(X_1, \cdots, X_n)h_{m-i}(X_1, X_2, \cdots, X_n) = 0. \tag{2.27}$$

Therefore, we have the following recurrence relation for $Q_k(j)$:

$$Q_k(j) = -\sum_{i=1}^{k} q_i(j)Q_{k-i}(j), \ k \geq 1. \tag{2.28}$$

Recall the generalized binomial coefficient for $k \in \mathbb{N}$, $z \in \mathbb{C}$

$$\binom{z}{k} = \frac{z(z-1)\cdots(z-k+1)}{k!}.$$

Lemma 3. *We have*

$$G_N = \sum_{m=0}^{[N/2]} G(N, m)\alpha^m, \quad N = 0, 1, 2, ...$$

where

$$G(N, m) = \binom{j}{m} Q_{N-2m}(j). \tag{2.29}$$

Moreover,

$$H_N = \sum_{m=0}^{[N/2]} H(N,m)\alpha^m, \quad N = 0, 1, 2, ...$$

where

$$H(N,m) = (-1)^N \binom{1-j}{m} q_{N-2m}(j). \tag{2.30}$$

Proof. Since

$$\prod_{i=0}^{j-1} \frac{1}{1+ix} = \sum_{i=0}^{\infty} Q_k(j)x^k, \tag{2.31}$$

we have

$$G(\alpha; x) = \sum_{m=0}^{j} \binom{j}{m} \alpha^m x^{2m} \sum_{k=0}^{\infty} Q_k(j)x^k = \sum_{N=0}^{\infty} x^N \sum_{m=0}^{[N/2]} \binom{j}{m} Q_{N-2m}(j)\alpha^m.$$

Similarly,

$$\begin{aligned} H(\alpha; x) &= \sum_{m=0}^{\infty} \binom{1-j}{m} \alpha^m x^{2m} \sum_{k=0}^{\infty} q_k(j)(-x)^k \\ &= \sum_{N=0}^{\infty} x^N \sum_{m=0}^{[N/2]} (-1)^N q_{N-2m}(j) \binom{1-j}{m} \alpha^m. \quad \square \end{aligned}$$

For fixed n, both $q_n(j)$ and $Q_n(j)$ are polynomials in j. Hence they can be naturally extended to be two functions defined on the whole real line. The following lemma gives a relation between these two functions.

Lemma 4. *For $n \geq 0$, we have $Q_n(1-t) = (-1)^n q_n(t)$, $t \in \mathbb{R}$.*

Proof. We denote for $j \geq 1$,

$$\phi_j(x) := \prod_{i=0}^{j-1} \frac{1}{1+ix} = \sum_{n=0}^{\infty} Q_n(j)x^n, \tag{2.32}$$

$$\psi_j(x) := \prod_{i=1}^{j-1} (1-ix) = \sum_{n=0}^{\infty} (-1)^n q_n(j)x^n. \tag{2.33}$$

In particular, $\phi_1(x) = \psi_1(x) = 1$. Note that

$$\phi_j(x) = (1+jx)\phi_{j+1}(x) = \sum_{n=0}^{\infty} \big(Q_n(j+1) + jQ_{n-1}(j+1)\big)x^n \tag{2.34}$$

where we set $Q_{-1}(t) = 0$. Comparing the coefficient of x^n on both sides, we deduce that for any $n \geq 0$,

$$Q_n(j) = Q_n(j+1) + jQ_{n-1}(j+1). \tag{2.35}$$

Similarly, observing that $\psi_{j+1}(x) = \psi_j(x)(1 - jx)$, we deduce that for any $n \geq 0$,

$$q_n(j+1) = q_n(j) + jq_{n-1}(j) \tag{2.36}$$

where we set $q_{-1}(t) = 0$. Since (2.35) and (2.36) hold for all $j \geq 1$ and both $Q_n(t)$ and $q_n(t)$ are polynomials in t, we conclude that for any $t \in \mathbb{R}$

$$Q_n(t) = Q_n(t+1) + tQ_{n-1}(t+1), \tag{2.37}$$

$$q_n(t+1) = q_n(t) + tq_{n-1}(t). \tag{2.38}$$

Now we let $\overline{Q}_n(t) = Q_n(1-t)$. Then (2.37) implies

$$\overline{Q}_n(t+1) = \overline{Q}_n(t) - t\overline{Q}_{n-1}(t). \tag{2.39}$$

Comparing (2.39) with (2.38), we see that the polynomials $\overline{Q}_n(t)$ and $(-1)^n q_n(t)$ satisfy the same recurrence relation. Next, by direct computation, we find that

$$Q_0(j) = q_0(j) = 1, \quad Q_1(j) = -\frac{j(j-1)}{2}, \quad q_1(j) = \frac{j(j-1)}{2}. \tag{2.40}$$

Thus

$$\overline{Q}_1(t) = -q_1(t) = -\frac{t(t-1)}{2}.$$

Now suppose that $\overline{Q}_{n-1}(t) = (-1)^{n-1} q_{n-1}(t)$ for some $n \geq 2$. By (2.38) and (2.39) we deduce that

$$\overline{Q}_n(t+1) - \overline{Q}_n(t) = (-1)^n q_n(t+1) - (-1)^n q_n(t).$$

Summing over t from 1 to $j - 1$, we obtain

$$\overline{Q}_n(j) - \overline{Q}_n(1) = (-1)^n q_n(j) - (-1)^n q_n(1). \tag{2.41}$$

By definition, we have $Q_n(1) = (-1)^n q_n(1) = 0$ for $n \geq 1$. Therefore, (2.41) implies that $\overline{Q}_n(j) = (-1)^n q_n(j)$ for any $j \geq 1$. This implies that $\overline{Q}_n(t) = (-1)^n q_n(t)$ for any $t \in \mathbb{R}$. $\square$

Since $G_0 = H_0$, $G_1 = H_1$, we get

$$\frac{G(\alpha(x);x) - H(\alpha(x);x)}{x^2} = \sum_{N=0}^{\infty} (G_{N+2} - H_{N+2}) x^N.$$

Hence

$$\frac{G(\alpha(x);x) - H(\alpha(x);x)}{x^2}(1 + \alpha(x)x^2) = \sum_{N=0}^{\infty} (G_{N+2} - H_{N+2} + (G_N - H_N)\alpha(x)) x^N. \tag{2.42}$$

To prove Lemma 2, we need to compute the coefficient of x^{n-1} in (2.42). For $N \geq 2m$, we define

$$\Delta(N,m) := G(N,m) - H(N,m) = \binom{j}{m} Q_{N-2m}(j) - (-1)^N \binom{1-j}{m} q_{N-2m}(j). \tag{2.43}$$

For example,

$$\begin{gathered}
\Delta(0,0) = \Delta(1,0) = 0, \\
\Delta(2,0) = \tfrac{1}{6} j(j-1)(2j-1), \quad \Delta(2,1) = 2j-1, \\
\Delta(3,0) = -\tfrac{1}{12}(j-1)^2 j^2 (2j-1), \quad \Delta(3,1) = -\tfrac{1}{2}(j-1)j(2j-1), \\
\Delta(4,0) = \tfrac{1}{240}(-1+j)j(-1+2j)(-4-12j+17j^2-10j^3+5j^4), \\
\Delta(4,1) = \tfrac{1}{24}(-1+j)j(-1+2j)(2-3j+3j^2), \quad \Delta(4,2) = 0, \\
\Delta(5,0) = -\tfrac{1}{1440}(-1+j)^2 j^2 (-1+2j)(-12-56j+61j^2-10j^3+5j^4), \\
\Delta(5,1) = -\tfrac{1}{48}(-1+j)^2 j^2 (-1+2j)(6-j+j^2), \quad \Delta(5,2) = 0.
\end{gathered}$$

Proposition 1. *Let $\mu = 2j - 1$ and $\nu = j(j-1)$. Then for $N \geq 2m$ the polynomial $\Delta(N,m)$ can be written as*

$$\Delta(N,m) = \mu(s_0 + s_1\nu + \cdots + s_k\nu^k), \quad s_0, s_1, \ldots, s_k \in \mathbb{Q}, \tag{2.44}$$

where $k \leq \left[\frac{2N-3m-1}{2}\right]$. Moreover, if $(N,m) \neq (2,1)$, then $s_0 = 0$.

In order to prove this proposition, we need the following lemmas.

Lemma 5. *Any polynomial of j can be written into a polynomial of $\mu = 2j - 1$ and $\nu = j(j-1)$, in which the degree of μ in each term is at most 1. Moreover, such a representation is unique. In order words, any polynomial $\varphi(j)$ can be uniquely written as*

$$\varphi(j) = s_{0,0} + s_{0,1}\nu + \dots + s_{0,n_0}\nu^{n_0} + \mu(s_{1,0} + s_{1,1}\nu + \dots + s_{1,n_1}\nu^{n_1}).$$

Furthermore, if all the coefficients of $\varphi(j)$ are rational numbers, then each $s_{i,l} \in \mathbb{Q}$.

Proof. Note that $\mu^2 = 4\nu + 1$. By the binomial theorem we have

$$\begin{aligned} j^n &= \left(\frac{\mu+1}{2}\right)^n = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\mu^k \\ &= 2^{-n}\left(\sum_{k=0}^{[n/2]}\binom{n}{2k}\mu^{2k} + \sum_{k=0}^{[(n-1)/2]}\binom{n}{2k+1}\mu^{2k+1}\right) \\ &= 2^{-n}\sum_{k=0}^{[n/2]}\binom{n}{2k}(4\nu+1)^k + 2^{-n}\mu\sum_{k=0}^{[(n-1)/2]}\binom{n}{2k+1}(4\nu+1)^k. \end{aligned} \tag{2.45}$$

This proves the assertions for the polynomial j^n.

Since any polynomial $\varphi(j)$ is a linear combinations of j^n $(n = 0, 1, \cdots)$, we know that $\varphi(j)$ can be written in the desired form. If $\varphi(j)$ has rational coefficients, then clearly each $s_{i,l} \in \mathbb{Q}$.

The uniqueness is clear, since otherwise we will have a relation

$$\varphi_1(\nu) + \mu\varphi_2(\nu) = 0$$

for some nonzero polynomials $\varphi_1(j)$ and $\varphi_2(j)$, which is impossible because $\mu^2 = 4\nu + 1$. $\square$

Remark 4. We see from (2.45) that $j^{2n} = \nu^n + \frac{n}{2}\mu\nu^{n-1}+$ lower degree terms and $j^{2n+1} = \frac{1}{2}\mu\nu^n+$ lower degree terms.

Lemma 6. *For $k \geq 1$,*

$$q_k(j) = \frac{1}{2^k k!}j^{2k} - \frac{2k+1}{3\cdot 2^k(k-1)!}j^{2k-1} + O(j^{2k-2}), \tag{2.46}$$

$$Q_k(j) = \frac{(-1)^k}{2^k k!}j^{2k} + \frac{(-1)^k(2k-5)}{3\cdot 2^k(k-1)!}j^{2k-1} + O(j^{2k-2}). \tag{2.47}$$

Proof. We denote

$$p_m(j) := \sum_{k=1}^{j-1} k^m. \tag{2.48}$$

It is known that

$$p_m(j) = \frac{1}{m+1}\sum_{i=0}^{m}(-1)^i\binom{m+1}{i}B_i j^{m+1-i} - j^m. \tag{2.49}$$

From (2.49) we have

$$p_1(j) = \frac{1}{2}j^2 - \frac{1}{2}j, \quad p_2(j) = \frac{1}{3}j^3 - \frac{1}{2}j^2 + \frac{1}{6}j.$$

As a polynomial in j, the degree of $p_m(j)$ is $m+1$. Moreover, it is known that

$$q_k(j) = (-1)^k \sum_{\substack{m_1+2m_2+\cdots+km_k=k\\ m_1\geq 0,\cdots,m_k\geq 0}} \prod_{i=1}^{k} \frac{(-p_i(j))^{m_i}}{m_i! i^{m_i}}. \tag{2.50}$$

As a polynomial in j, the degree of $q_k(j)$ is no more than

$$\begin{aligned}\deg\big(\prod_{i=1}^{k} p_i^{m_i}(j)\big) &= 2m_1 + 3m_2 + \cdots + (k+1)m_k\\ &= (m_1 + 2m_2 + \cdots + km_k) + (m_1 + m_2 + \cdots + m_k)\\ &= k + (m_1 + m_2 + \cdots + m_k)\\ &\leq 2k.\end{aligned}$$

Now we are going to find the coefficients of j^{2k} and j^{2k-1} in $q_k(j)$, respectively.

We consider the system of linear equations

$$\begin{cases} 2m_1 + 3m_2 + \cdots + (k+1)m_k = 2k\\ m_1 + 2m_2 + \cdots + km_k = k, \end{cases}$$

which is equivalent to

$$\begin{cases} m_1 + m_2 + \cdots + m_k = k\\ m_1 + 2m_2 + \cdots + km_k = k. \end{cases}$$

It is clear that the unique solution to the equations above are $m_1 = k$ and $m_i = 0$ for $2 \leq i \leq k$. Now we compute

$$\begin{aligned}(-1)^k\frac{(-p_1(j))^k}{k!} &= \frac{1}{k!}\left(\frac{1}{2}j^2 - \frac{1}{2}j\right)^k\\ &= \frac{1}{k!}\left(\frac{1}{2^k}j^{2k} - \frac{k}{2^k}j^{2k-1} + O(j^{2k-2})\right).\end{aligned} \tag{2.51}$$

Similarly, we consider the system of linear equations

$$\begin{cases} 2m_1 + 3m_2 + \cdots + (k+1)m_k = 2k-1 \\ m_1 + 2m_2 + \cdots + km_k = k. \end{cases}$$

The only solutions are $m_1 = k-2$, $m_2 = 1$ and $m_i = 0$ for all $i \geq 3$. The corresponding term in $q_k(j)$ is

$$\begin{aligned} (-1)^k \frac{(-p_1(j))^{k-2}}{(k-2)!} \cdot \frac{-p_2(j)}{2!} &= -\frac{1}{2(k-2)!}\left(\frac{1}{2}j^2 - \frac{1}{2}j\right)^{k-2} \cdot \left(\frac{1}{3}j^3 - \frac{1}{2}j^2 + \frac{1}{6}j\right) \\ &= -\frac{1}{3 \cdot 2^{k-1}(k-2)!} j^{2k-1} + O(j^{2k-2}). \end{aligned} \tag{2.52}$$

Adding (2.51) and (2.52) up, we obtain (2.46).

Next, from Lemma 4, we see that if we replace j by $1-j$ in the polynomial expression of $(-1)^k q_k(j)$, then we get $Q_k(j)$. Thus by replacing j by $1-j$ in (2.46), we obtain (2.47). □

Lemma 7. *For any integer $n \geq 1$, both $q_n(j)$ and $Q_n(j)$ are divisible by $j(j-1)$, and $q_{2n+1}(j)$ is divisible by $j^2(j-1)^2$.*

Proof. By definition we have $q_n(j) = Q_n(j) = 0$ when $j = 0$ and $j = 1$. As polynomials of j, we know that $q_n(j)$ and $Q_n(j)$ are divisible by $j(j-1)$.

Furthermore, from Newton's identities, we have

$$mq_m(j) = \sum_{k=1}^{m} (-1)^{k-1} p_k(j) q_{m-k}(j). \tag{2.53}$$

For each $1 \leq k \leq m-1$, $p_k(j)q_{m-k}(j)$ is divisible by $j^2(j-1)^2$. It is well known that if $m \geq 3$ is odd, then $p_m(j)$ is divisible by $j^2(j-1)^2$. Hence (2.53) implies that $q_{2n+1}(j)$ is divisible by $j^2(j-1)^2$ for any $n \geq 1$. □

Now we are able to prove Proposition 1.

Proof of Proposition 1. From (2.43) it is clear that $\Delta(N,m)$ is a polynomial of j with rational coefficients. By Lemma 5, we can write

$$\Delta(N,m) = s_{0,0} + s_{0,1}\nu + \cdots + s_{0,n_0}\nu^{n_0} + \mu\left(s_{1,0} + s_{1,1}\nu + \cdots + s_{1,n_1}\nu^{n_1}\right) \tag{2.54}$$

where each $s_{i,l} \in \mathbb{Q}$. Replacing j by $1-j$, then $\mu \mapsto -\mu$ and $\nu \mapsto \nu$. Lemma 4 and (2.43) imply

$$-\Delta(N,m) = s_{0,0} + s_{0,1}\nu + \cdots + s_{0,n_0}\nu^{n_0} - \mu\left(s_{1,0} + s_{1,1}\nu + \cdots + s_{1,n_1}\nu^{n_1}\right). \tag{2.55}$$

From (2.54) and (2.55), we deduce that

$$\Delta(N,m) = \mu\left(s_{1,0} + s_{1,1}\nu + \cdots + s_{1,n_1}\nu^{n_1}\right).$$

By Lemma 7 and (2.43) we know that $\Delta(N,m)$ is divisible by ν when $N-2m>0$. If $N-2m=0$, we have

$$\Delta(2m,m) = \binom{j}{m} - \binom{1-j}{m}.$$

Clearly, when $j=0$ or $j=1$, we have $\Delta(2m,m)=0$ except when $m=1$. Therefore $\Delta(2m,m)$ has a factor $j(j-1)$ except when $m=1$. Thus when $(N,m)\neq(2,1)$, $\Delta(N,m)$ is always divisible by ν, which means $s_{1,0}=0$.

It remains to prove that $n_1 \leq \left[\frac{2N-3m-1}{2}\right]$. By the definition of $G(N,m)$ and Lemma 6,

$$G(N,m) = \frac{(-1)^N}{m!(N-2m)!2^{N-2m}} j^{2N-3m} + O(j^{2N-3m-1}). \tag{2.56}$$

Similarly,

$$H(N,m) = \frac{(-1)^{N-m}}{m!(N-2m)!2^{N-2m}} j^{2N-3m} + O(j^{2N-3m-1}). \tag{2.57}$$

Hence

$$\Delta(N,m) = \text{Const. } \mu\nu^{\left[\frac{2N-3m-1}{2}\right]} + \text{lower degree terms}. \tag{2.58}$$

This completes the proof of Proposition 1. □

Finally, we arrive at the stage to prove Lemma 2.

Proof of Lemma 2. We plug

$$\alpha(x) = \sum_{k=0}^{\infty} a_k x^k$$

into (2.42) and expand it to a power series of x. By direct calculations, we find that the coefficient of x^{n-1} in (2.42) is the sum of the following terms:

$$\Delta(2,1)a_{n-1}, \tag{2.59}$$

$$(\Delta(N,m) + \Delta(N-2,m-1)) \sum_{i_1+\ldots+i_m=n-N+1} a_{i_1}\cdots a_{i_m} \tag{2.60}$$

$(3 \leq N \leq n+1,\ 1 \leq m \leq [\frac{N}{2}])$,

$$\Delta(n+1,0). \tag{2.61}$$

Note that $\Delta(2,1) = 2j - 1 = \mu$. (2.59) gives the first term in (2.19). By Proposition 1, we can write each $\Delta(N,m)$ as

$$\mu(s_0 + s_1\nu + ... + s_k\nu^k), \quad s_0, s_1, \dots, s_k \in \mathbb{Q},$$

where $k \le [\frac{2N-3m-1}{2}]$. Since $N \le n+1$, $m \ge 0$, we have $[\frac{2N-3m-1}{2}] \le n$, which means the degree of ν in $\Delta(N,m)$ is at most n. This gives (2.19) and clearly each polynomial $S_i(n)$ has rational coefficients. More explicitly, from (2.60) and (2.61), we see that for $i = 0, 1, ..., n$,

$$\begin{aligned} &S_i(n) = [\mu\nu^i]\Delta(n+1,0) \\ &+ \sum_{N=3}^{n+1}\sum_{m=1}^{[N/2]}\sum_{i_1+\ldots+i_m=n-N+1}([\mu\nu^i]\Delta(N,m) + [\mu\nu^i]\Delta(N-2,m-1))a_{i_1}\cdots a_{i_m}, \end{aligned} \tag{2.62}$$

where $[\mu\nu^i]\Delta(N,m)$ means the coefficient of the term $\mu\nu^i$ in $\Delta(N,m)$. In particular,

$$S_i(1) = [\mu\nu^i]\Delta(2,0), \quad i = 0, 1,$$
$$S_i(2) = [\mu\nu^i]\Delta(3,0) + [\mu\nu^i]\Delta(3,1)a_0, \quad i = 0, 1, 2.$$

Recall that $\Delta(2,0) = \frac{1}{6}\mu\nu$, $\Delta(3,0) = -\frac{1}{12}\mu\nu^2$, and $\Delta(3,1) = -\frac{1}{2}\mu\nu$. So we have $S_0(1) = S_0(2) = 0$, $S_1(1) = \frac{1}{6}$, $S_1(2) = -\frac{1}{2}a_0$, $S_2(2) = -\frac{1}{12}$. $\square$

3. Proof of Theorem 1

Recall Ramanujan's Theta-operator $\Theta = q\partial_q$, which has the effect that

$$\Theta\left(\sum_{n=n_0}^{\infty} x(n)q^n\right) := \sum_{n=n_0}^{\infty} nx(n)q^n.$$

Let

$$P_0 = \sum_{j=1}^{\infty}(-1)^{j-1}(2j-1)q^{j(j-1)/2}.$$

Lemma 8. *For any $m \ge 1$, we have*

$$\Theta^m(P_0) = -3P_0P_m,$$

where P_m is a multivariate polynomial of $A_0, A_1, ..., A_{m-1}$ with rational coefficients and A_i was defined in (1.8). Moreover, we have

$$P_1 = A_0, \quad P_{m+1} = \Theta(P_m) - 3A_0P_m, \ m = 1, 2, \dots.$$

Proof. By Jacobi's identity [1, Theorem 1.3.9], we have

$$P_0 = \prod_{n=1}^{\infty}(1-q^n)^3. \tag{3.1}$$

Hence

$$\frac{\Theta(P_0)}{P_0} = -3\sum_{n=1}^{\infty}\frac{nq^n}{1-q^n} = -3\sum_{n=1}^{\infty}\sigma(n)q^n.$$

This proves that $\Theta(P_0) = -3A_0P_0$ and hence $P_1 = A_0$.

Next, note that

$$\Theta^{m+1}(P_0) = \Theta(-3P_0P_m) = -3\Theta(P_0)P_m - 3P_0\Theta(P_m) = -3P_0(\Theta(P_m) - 3A_0P_m).$$

We deduce that

$$P_{m+1} = \Theta(P_m) - 3A_0P_m. \tag{3.2}$$

Suppose we have proved that P_m is a polynomial of A_0, A_1, $\dots$, A_{m-1} with rational coefficients, which is clearly true for $m = 1$. Then since $\Theta(A_k) = A_{k+1}$, from (3.2) it follows that P_{m+1} is a polynomial of A_0, A_1, $\dots$, A_m with rational coefficients. Thus by induction on m we know that the first assertion is true. □

Recall that in Lemma 2, $S_0(1) = 0$, $S_1(1) = \frac{1}{6}$, and for $m \geq 2$, $S_i(m)$ are polynomials of a_0, a_1, $\cdots$, a_{m-2} and independent of j. For $m \geq 1$, we recursively define

$$C_m = -S_0(m) + \sum_{i=1}^{m} 3\cdot 2^i S_i(m)(C_1,\cdots,C_{m-1})P_i. \tag{3.3}$$

In particular,

$$C_1 = 6S_1(1)P_1 = A_0. \tag{3.4}$$

The following lemma is a key for the proof of Theorem 1.

Lemma 9. *Let $n \geq 1$ and $\lambda \neq C_n$. In addition, we assume $\lambda > 0$ when $n = 1$. Then for large k,*

$$(-1)^k(\lambda - C_n)f(-(k + \Lambda_{n-1}(k^{-1})k^{-1})q^{1-k}) > 0, \tag{3.5}$$

where

$$\Lambda_{n-1}(x) = \sum_{i=1}^{n-1} C_i x^{i-1} + \lambda x^{n-1}. \tag{3.6}$$

Remark 5. Here and in the proof below, we use the convention that in any summation $\sum_{i=a}^{b}$, if $a > b$, then we assume the sum is empty (zero). In (3.6), when $n = 1$, we have an empty sum and so $\Lambda_0(x) = \lambda$.

Proof. For convenience, we define for $m \geq 0$

$$\overline{P}_m := \sum_{j=1}^{\infty} (-1)^{j-1}(2j-1)\,(j(j-1))^m\, q^{j(j-1)/2} \tag{3.7}$$

and

$$\overline{P}_{m,2N-1} := \sum_{j=1}^{2N-1} (-1)^{j-1}(2j-1)\,(j(j-1))^m\, q^{j(j-1)/2}. \tag{3.8}$$

It is clear that $\overline{P}_0 = P_0$ and $\overline{P}_m = 2^m \Theta^m(P_0) = -3 \cdot 2^m P_0 P_m$ $(m \geq 1)$. Moreover, (3.3) implies that for any $m \geq 1$,

$$C_m P_0 + \sum_{i=0}^{m} S_i(m)(C_1, C_2, \cdots, C_{m-1})\overline{P}_i = 0. \tag{3.9}$$

Since q is fixed with $0 < q < 1$, we have $\Lambda_0(k^{-1}) = \lambda > 0$ and $\Lambda_{n-1}(k^{-1}) = C_1 + O(k^{-1})$ for $n \geq 2$. Note that $C_1 = A_0 = \sum_{m=1}^{\infty} \sigma(m) q^m > 0$. Now we set $a = \Lambda_{n-1}(x)$ in (2.1) with $x = k^{-1}$. From (2.13) and Lemma 2 we deduce that

$$\begin{aligned} v_{k-j} =& \Big(G(\Lambda_{n-1}(k^{-1}); k^{-1}) - H(\Lambda_{n-1}(k^{-1}); k^{-1}) \Big) \frac{1 + \Lambda_{n-1}(k^{-1})k^{-2}}{k^{-2}} q^{j(j-1)/2} \\ & \cdot (k + \Lambda_{n-1}(k^{-1})k^{-1})^{k-2} \frac{1}{k!} q^{-k(k-1)/2} \\ =& (k + \Lambda_{n-1}(k^{-1})k^{-1})^{k-2} \frac{1}{k!} q^{-k(k-1)/2} \cdot q^{j(j-1)/2} \Big(\sum_{m=1}^{n} \xi_{m-1} k^{-(m-1)} + O(k^{-n}) \Big), \end{aligned} \tag{3.10}$$

where

$$\xi_{m-1} = \mu \left(C_m + \sum_{i=0}^{m} S_i(m)(C_1, \cdots, C_{m-1}) \nu^i \right), \quad 1 \leq m \leq n-1, \tag{3.11}$$

and

$$\xi_{n-1} = \mu \left(\lambda + \sum_{i=0}^{n} S_i(n)(C_1, \cdots, C_{n-1}) \nu^i \right). \tag{3.12}$$

For convenience, from now to the end of proof, we will omit the variables $C_1, \cdots, C_{n-1}$ and simply write the polynomial $S_i(j)(C_1, \cdots, C_{j-1})$ as $S_i(j)$.

By Lemma 1, there exists a positive integer $N_1 = N_1(q)$ such that for $k \geq q^{-3N_1}$,

$$v_{k-N_1} > v_{k-N_1-1} > \cdots > v_0.$$

Note that (3.1) implies $P_0 > 0$. If $\lambda - C_n < 0$, by (3.9) we know there exists a positive integer $N_2 = N_2(q)$ such that for any integers $m \geq N_2$,

$$\lambda \overline{P}_{0,2m-1} + \sum_{i=0}^{n} S_i(n) \overline{P}_{i,2m-1} < 0. \tag{3.13}$$

Let $N > \max\{N_1, N_2\}$. Using (3.10) and by direct calculations, we find that

$$\begin{aligned} &\sum_{j=1}^{2N-1} (-1)^{j-1} v_{k-j} = \\ &(k + \Lambda_{n-1}(k^{-1})k^{-1})^{k-2} \frac{1}{k!} q^{-k(k-1)/2} \cdot \Bigg(\sum_{\ell=1}^{n-1} \big(C_\ell \overline{P}_{0,2N-1} + \sum_{i=0}^{\ell} S_i(\ell) \overline{P}_{i,2N-1}\big) k^{-(\ell-1)} \\ &+ \big(\lambda \overline{P}_{0,2N-1} + \sum_{i=0}^{n} S_i(n) \overline{P}_{i,2N-1}\big) k^{-(n-1)} + O(k^{-n}) \Bigg). \end{aligned} \tag{3.14}$$

Now for each $1 \leq \ell \leq n-1$, from (3.9) we deduce that

$$C_\ell \overline{P}_0 + \sum_{i=0}^{\ell} S_i(\ell) \overline{P}_i = 0. \tag{3.15}$$

Hence

$$\begin{aligned} &\left| \left(C_\ell \overline{P}_{0,2N-1} + \sum_{i=0}^{\ell} S_i(\ell) \overline{P}_{i,2N-1} \right) k^{-(\ell-1)} \right| \\ =& \left| \sum_{j \geq 2N} \big(C_\ell + \sum_{i=0}^{\ell} S_i(\ell) v^i \big) (-1)^{j-1} (2j-1) q^{j(j-1)/2} \right| \\ \leq& |C_\ell| \left| \sum_{j \geq 2N} (-1)^{j-1} (2j-1) q^{j(j-1)/2} \right| \\ &+ \sum_{i=0}^{\ell} |S_i(\ell)| \left| \sum_{j \geq 2N} (-1)^{j-1} (2j-1) (j(j-1))^i q^{j(j-1)/2} \right| \end{aligned}$$

$$\leq |C_\ell|(4N-1)q^{N(2N-1)} + \sum_{i=0}^{\ell} |S_i(\ell)|(4N-1)(2N(2N-1))^i q^{N(2N-1)}$$

$$= O(q^{N^2}).$$

Here for the last inequality, we have used the fact that when N is sufficiently large, the sequence $(2j-1)(j(j-1))^i q^{j(j-1)/2}$ will be decreasing when $j \geq 2N$.

Note that when $k \leq q^{-N^2/n}$, we have $q^{N^2} \leq k^{-n}$. Hence for each k satisfying $q^{-3N} \leq k \leq q^{-N^2/n}$, (3.14) implies

$$\sum_{j=1}^{2N-1} (-1)^{j-1} v_{k-j} = (k + \Lambda_{n-1}(k^{-1})k^{-1})^{k-2} \frac{1}{k!} q^{-k(k-1)/2} \times \left(\left(\lambda \overline{P}_{0,2N-1} + \sum_{i=0}^{n} S_i(n) \overline{P}_{i,2N-1} \right) k^{-(n-1)} + O(k^{-n}) \right). \tag{3.16}$$

From (3.13), when N is large enough, and for k satisfying $q^{-3N} \leq k \leq q^{-N^2/n}$, we can guarantee that

$$\left(\lambda \overline{P}_{0,2N-1} + \sum_{i=0}^{n} S_i(n) \overline{P}_{i,2N-1} \right) k^{-(n-1)} + O(k^{-n}) < 0. \tag{3.17}$$

Therefore, for such k and N, we have

$$\sum_{j=1}^{2N-1} (-1)^{j-1} v_{k-j} < 0 \tag{3.18}$$

and by Lemma 1

$$\sum_{j=2N}^{k} (-1)^{j-1} v_{k-j} < v_{k-2N-1} - v_{k-2N} < 0. \tag{3.19}$$

So we have

$$(-1)^k \sum_{n=0}^{2k-1} (-1)^n u_n = \sum_{j=1}^{k} (-1)^{j-1} v_{k-j} < 0. \tag{3.20}$$

By (3.17) we know that there exists a constant $c > 0$ such that for k large enough,

$$\left| \sum_{n=0}^{2k-1} (-1)^n u_n \right| > c \frac{(k + \Lambda_{n-1}(k^{-1})k^{-1})^{k-2}}{k!} q^{-k(k-1)/2} k^{-(n-1)}$$

$$> \frac{(k+\Lambda_{n-1}(k^{-1})k^{-1})^{2k}}{(2k)!}q^k = u_{2k}. \tag{3.21}$$

Moreover, since u_n is decreasing when $n > k$,

$$u_{2k} > \left|\sum_{n=2k}^{\infty} u_n(-1)^n\right|. \tag{3.22}$$

From (3.20), (3.21) and (3.22), we deduce that

$$(-1)^k f(-(k+\Lambda_{n-1}(k^{-1})k^{-1})q^{1-k}) = \sum_{n=0}^{\infty}(-1)^n u_n < 0$$

for large k.

Similarly, if $\lambda - C_n > 0$, we have for large k,

$$(-1)^k f(-(k+\Lambda_{n-1}(k^{-1})k^{-1})q^{1-k}) > 0. \quad \square$$

Proof of Theorem 1. For any $n \geq 1$, we choose $\lambda' < C_n < \lambda''$ where we also require that $\lambda' > 0$ when $n = 1$. Let

$$\xi_k' = -kq^{1-k}\left(1 + \sum_{i=1}^{n-1} C_i k^{-1-i} + \lambda' k^{-1-n}\right),$$
$$\xi_k'' = -kq^{1-k}\left(1 + \sum_{i=1}^{n-1} C_i k^{-1-i} + \lambda'' k^{-1-n}\right).$$

By Lemma 9 we have $f(\xi_k')f(\xi_k'') < 0$. Therefore, by the intermediate value theorem, there exists a root in the interval $(\xi_k',\ \xi_k'')$. Thanks to (1.5), when k is large enough, we know this interval contains only one root and this root must be x_k (see also [25, Proof of Theorem 1]). Thus we can write the root as

$$x_k = -kq^{1-k}\left(1 + \sum_{i=1}^{n-1} C_i k^{-1-i} + \theta_n(k) k^{-1-n}\right). \tag{3.23}$$

By letting λ' and λ'' tend to C_n from the left side and right side, respectively, we see that we must have

$$\lim_{k\to\infty} \theta_n(k) = C_n. \tag{3.24}$$

Thus $\theta_n(k) = C_n + o(1)$ as k tends to infinity. This means

$$x_k = -kq^{1-k}\left(1 + \sum_{i=1}^{n-1} C_i k^{-1-i} + C_n k^{-1-n} + o(k^{-1-n})\right). \tag{3.25}$$

This proves (1.9) for any $n \geq 1$.

From the definition (3.3) and Lemma 8, it is clear that C_i is a multivariate polynomial of A_0, A_1, ..., A_{i-1} with rational coefficients. □

4. Representations of C_n

4.1. Representation of C_n using $A_0, A_1, \cdots, A_{n-1}$

We have seen in (3.3) that

$$C_n = -S_0(n) + 6S_1(n)P_1 + 12S_2(n)P_2 + ... + 3 \cdot 2^n S_n(n)P_n, \tag{4.1}$$

where each P_i is given by a recursive formula in Lemma 8, and each $S_i(n)$ can be determined from (2.62) by setting $a_i = C_{i+1}$. Indeed, for $i = 0, 1, ..., n$,

$$S_i(n) = [\mu\nu^i]\Delta(n+1, 0) + \sum_{N=3}^{n+1} \sum_{m=1}^{[N/2]} \sum_{i_1+...+i_m=n-N+m+1} ([\mu\nu^i]\Delta(N, m) + [\mu\nu^i]\Delta(N-2, m-1))C_{i_1} \cdots C_{i_m}, \tag{4.2}$$

where $\Delta(N, m)$ was given in (2.43), and $[\mu\nu^i]\Delta(N, m)$ means the coefficient of the term $\mu\nu^i$ in the representation of $\Delta(N, m)$ in Proposition 1.

Proposition 2. *For $n \geq 1$,*

$$S_n(n) = \frac{(-1)^{n-1}}{3 \cdot 2^n (n-1)!}.$$

Proof. By Lemma 6, (2.29) and (2.30) we have

$$G(N, 0) = Q_N(j) = \frac{(-1)^N}{2^N N!} j^{2N} + \frac{(-1)^N (2N-5)}{3 \cdot 2^N (N-1)!} j^{2N-1} + O(j^{2N-2}),$$
$$H(N, 0) = (-1)^N q_N(j) = \frac{(-1)^N}{2^N N!} j^{2N} - \frac{(-1)^N (2N+1)}{3 \cdot 2^N (N-1)!} j^{2N-1} + O(j^{2N-2}).$$

Then by (2.43) we have

$$\Delta(N, 0) = \frac{(-1)^N}{3 \cdot 2^{N-2} (N-2)!} j^{2N-1} + O(j^{2N-2}). \tag{4.3}$$

So

$$\Delta(n+1, 0) = \frac{(-1)^{n+1}}{3 \cdot 2^n (n-1)!} \mu\nu^n + \text{lower degree terms}. \tag{4.4}$$

Thanks to (2.58), we know that in (4.2), $\Delta(n+1,0)$ is the only term containing $\mu\nu^n$, so $S_n(n)$ is exactly the coefficient of $\mu\nu^n$ in (4.4). □

Proposition 3. *For $n \geq 3$,*

$$S_0(n) = \sum_{i_1+i_2=n-1} C_{i_1}C_{i_2}.$$

Proof. Recall that $S_0(n) = 0$ if $n = 1,\ 2$. From Proposition 1 we know that when $n \geq 3$, any other $\Delta(N, m)$ with $(N, m) \neq (2, 1)$ in (4.2) must have the factor $\mu\nu$. Recall that $\Delta(2, 1) = \mu$. So

$$S_0(n) = [\mu]\Delta(2,1) \sum_{i_1+i_2=n-1} C_{i_1}C_{i_2} = \sum_{i_1+i_2=n-1} C_{i_1}C_{i_2}. \quad \square$$

Proposition 4. *For $1 \leq i \leq n-1$, $S_i(n)$ is a polynomial of $C_1, ..., C_{n-i}$ with degree $\leq \min\{[\frac{2(n-i)+1}{3}], [\frac{n+1}{2}]\}$. Moreover, this polynomial has the form*

$$\tilde{F}(C_1, ..., C_{n-i-1}) + \frac{(-1)^i}{2^i i!}C_{n-i}, \tag{4.5}$$

when $\tilde{F}$ is a polynomial depending on n and i.

Proof. To show that the subscripts of C_k's in S_i are at most $n-i$, we need to analyze the terms associated with each $[\mu\nu^i]\Delta(N, m)$ in (4.2). Recall that (2.58) gives the restriction $[\frac{2N-3m-1}{2}] \geq i$ on these (N, m). We consider two different cases. When $m \geq 1$, we have $N - 2 \geq [\frac{2N-3m-1}{2}] \geq i$, so $N \geq i + 2$. The term associated with $[\mu\nu^i]\Delta(N, m)$ is

$$\sum_{i_1+...+i_m=n-N+m+1} C_{i_1}...C_{i_m} + \sum_{i_1+...+i_{m+1}=n-N+m} C_{i_1}...C_{i_{m+1}}. \tag{4.6}$$

(Note that when $N = n,\ n + 1$, the second sum vanishes.) So the maximal subscript

$$\max_l i_l \leq n - N_{\min} + 2 = n - i.$$

When $m = 0$, the term associated with $[\mu\nu^i]\Delta(N, 0)$ is C_{n-N} if $N \leq n-1$, is 0 if $N = n$, and is 1 if $N = n+1$. Since $N - 1 = [\frac{2N-3m-1}{2}] \geq i$, we have $N \geq i+1$. So the subscript

$$n - N \leq n - N_{\min} = n - i - 1 < n - i.$$

Consequently, $S_i(n)$ contains only $C_1, ..., C_{n-i}$.

Since $[\frac{2N-3m-1}{2}] \geq i$, we have $m \leq [\frac{2N-2i-1}{3}]$. The degree of (4.6), as a polynomial of $C_1, ..., C_{n-i}$, is $m + 1$ when $N \leq n - 1$, and is m when $N = n,\ n + 1$. When $N \leq n - 1$,

$$m + 1 \leq [\tfrac{2(n-1)-2i-1}{3}] + 1 = [\tfrac{2(n-i)}{3}].$$

When $N = n,\ n+1$,

$$m \le [\tfrac{2(n+1)-2i-1}{3}] = [\tfrac{2(n-i)+1}{3}].$$

Recall that $m \le [N/2]$. So the degree of $S_i(n)$, as a polynomial of $C_1, ..., C_{n-i}$, is at most $\min\{[\frac{2(n-i)+1}{3}], [\frac{n+1}{2}]\}$.

The coefficient of C_{n-i} in (4.2) is $[\mu\nu^i]\Delta(i+2,1)+[\mu\nu^i]\Delta(i,0)$. By (2.56), (2.57), and (4.3), we have

$$\Delta(i+2,1) = \frac{(-1)^i}{2^i i!}\mu\nu^i + \text{lower degree terms},$$

$$\Delta(i,0) = \frac{(-1)^i}{3\cdot 2^{i-1}(i-2)!}\mu\nu^{i-1} + \text{lower degree terms},$$

which implies $[\mu\nu^i]\Delta(i+2,1)+[\mu\nu^i]\Delta(i,0) = \frac{(-1)^i}{2^i i!}$. $\square$

Proposition 5. *For any $n \ge 1$,*

$$C_n = F(A_0, ..., A_{n-2}) + \frac{(-1)^{n-1}}{(n-1)!}A_{n-1}, \tag{4.7}$$

where F is a polynomial depending on n and has degree at most n.

Proof. From the definition of P_n in Lemma 8, one can prove by induction that for any $n \ge 1$, the degree of the multivariate polynomial P_n is n, and

$$P_n = A_{n-1} + \text{higher degree terms (without } A_{n-1}). \tag{4.8}$$

So the coefficient of A_{n-1} in C_n is exactly $\frac{(-1)^{n-1}}{(n-1)!}$ by (4.1) and Proposition 2. To show the degree of C_n is at most n, we use induction. Suppose $\deg(C_l) \le l$, $1 \le l < n$. Then one can estimate the degree of C_n directly by (4.1) and (4.2). For example, the term

$$[\mu\nu^i]\Delta(N,m)P_i \sum_{i_1+...+i_m=n-N+m+1} C_{i_1}\cdots C_{i_m}$$

has degree at most

$$\Big[\frac{2N-3m-1}{2}\Big] + (n-N+m+1) = \Big[n - \frac{1}{2}m + \frac{1}{2}\Big] \le n.$$

Other terms can be estimated similarly. So $\deg(C_n) \le n$. $\square$

4.2. The linear terms in the representation of C_n

We have known that C_n is a multivariate polynomial of $A_0, ..., A_{n-1}$, which has the form (4.7) and can be determined recursively by (4.1). However, from the examples presented in Section 1, we see that this multivariate polynomial may have a very complicated structure, since it contains nonlinear terms as well as linear terms. In this section, we will see that at least the linear terms can be understood.

For $i = 1, ..., n$, let $S_{i,0}(n)$ be the constant term in $S_i(n)$. By (4.2), we have

$$\Delta(n+1,0) = Q_{n+1}(j) - (-1)^{n+1}q_{n+1}(j) = S_{n,0}(n)\mu\nu^n + ... + S_{2,0}(n)\mu\nu^2 + S_{1,0}(n)\mu\nu.$$

Then by (4.8) and (4.1), the coefficient of the linear term A_{i-1} in C_n equals to

$$3 \cdot 2^i S_{i,0}(n).$$

We have obtained the coefficient of the linear term A_{n-1} in Proposition 5. However, to determine the explicit formulas of the coefficients for other linear terms, we have to obtain the explicit expansion of $q_{n+1}(j)$ (i.e., the unsigned Stirling number of the first kind $c(j, j-n-1)$). Although it is possible to determine the first several terms in the expansions (see Lemma 6 for the first two terms), complete expansions are difficult and unknown. Fortunately, the sum of these coefficients has a simple closed form, which gives the coefficient of q in the expansion of $C_n(q)$ in q (see Remark 3).

Proposition 6. *The sum of the coefficients of the linear terms $A_0, A_1, ..., A_{n-1}$ in C_n equals to $(-1)^{n-1}$.*

Proof. The sum of the coefficients of the linear terms $A_0, A_1, ..., A_{n-1}$ in C_n equals to

$$6S_{1,0}(n) + 12S_{2,0}(n) + ... + 3 \cdot 2^n S_{n,0}(n). \tag{4.9}$$

Note that

$$\Delta(n+1,0) = S_{n,0}(n)\mu\nu^n + ... + S_{2,0}(n)\mu\nu^2 + S_{1,0}(n)\mu\nu. \tag{4.10}$$

To compute the value of (4.9), we only need to set $\mu = 3$ and $\nu = 2$, namely $j = 2$ in (4.10). Note that when $j = 2$

$$G(N,0) = (-1)^N, \quad H(N,0) = 0, \quad N = 2, 3, ...$$

So $\Delta(n+1,0) = G(n+1,0) - H(n+1,0) = (-1)^{n+1}$. □

Although it is difficult to find $S_{i,0}(n)$ for all $0 \le i \le n$, we are able to find explicit formulas for $S_{1,0}(n)$ and $S_{2,0}(n)$, which give us explicit formulas for the coefficients of the linear terms A_0 and A_1. These results are useful in proving Theorem 2.

Proposition 7. *For any $n \geq 1$,*

$$S_{1,0}(2n) = 0, \quad S_{1,0}(2n-1) = \frac{B_{2n}}{n}, \quad S_{2,0}(2n) = -\frac{B_{2n}}{2n}. \tag{4.11}$$

Proof. Since $\Delta(n,0) = Q_n(j) - (-1)^n q_n(j)$, we have $Q_n(j) = \Delta(n,0) + (-1)^n q_n(j)$. By (2.28) we have

$$(-1)^n q_n(j) + \Delta(n,0) = -\sum_{m=0}^{n-1} q_{n-m}(j)\left((-1)^m q_m(j) + \Delta(m,0)\right).$$

This implies

$$\Delta(n,0) = -\sum_{m=0}^{n-1} \Delta(m,0) q_{n-m}(j) - \sum_{m=0}^{n} (-1)^m q_m(j) q_{n-m}(j). \tag{4.12}$$

Note that for any $n \geq 1$, $q_n(j)$ is divisible by $\nu = j(j-1)$. Since $\Delta(0,0) = \Delta(1,0) = 0$, from (4.12), we know $\Delta(n,0)$ is divisible by ν. Replacing n by $2n+1$ in (4.12) and observing that

$$\begin{aligned} &\sum_{m=0}^{2n+1} (-1)^m q_m(j) q_{2n+1-m}(j) \\ &= \sum_{m=0}^{n} \left((-1)^m q_m(j) q_{2n+1-m}(j) + (-1)^{2n+1-m} q_{2n+1-m}(j) q_m(j)\right) \\ &= 0, \end{aligned}$$

we obtain

$$\Delta(2n+1,0) = -\sum_{m=0}^{2n} \Delta(m,0) q_{2n+1-m}(j). \tag{4.13}$$

Since both $\Delta(m,0)$ and $q_{2n+1-m}(j)$ are divisible by ν, we know that $\Delta(2n+1,0)$ is divisible by ν^2. Therefore, from (4.10) we know $S_{1,0}(2n) = 0$.

Now we compare the coefficients of $\mu\nu^2$ in both sides of (4.13). For the left hand side, it is clearly equal to $S_{2,0}(2n)$. For the right hand side, if $0 \leq m \leq 2n-1$ is odd, then $\Delta(m,0)$ is divisible by ν^2 and $q_{2n+1-m}(j)$ is divisible by ν. If $0 \leq m \leq 2n-1$ is even, then $\Delta(m,0)$ is divisible by ν and $q_{2n+1-m}(j)$ is divisible by ν^2 (see Lemma 7). Hence for any $0 \leq m \leq 2n-1$, $\Delta(m,0)q_{2n+1-m}(j)$ is always divisible by ν^3. Thus the term $\mu\nu^2$ only appears in $\Delta(2n,0)q_1(j)$, and hence equals to $-\frac{1}{2}S_{1,0}(2n-1)\mu\nu^2$. Thus we obtain

$$S_{2,0}(2n) = -\frac{1}{2} S_{1,0}(2n-1). \tag{4.14}$$

Now we determine $S_{1,0}(2n-1)$. Replacing n by $2n$ in (4.12), we obtain

$$\Delta(2n,0) = -2q_{2n}(j) - \sum_{m=1}^{2n-1}(-1)^m q_m(j)q_{2n-m}(j) - \sum_{m=0}^{2n-1}\Delta(m,0)q_{2n-m}(j). \quad (4.15)$$

Comparing the coefficient of j on both sides, we obtain

$$S_{1,0}(2n-1) = -2[j]q_{2n}(j). \quad (4.16)$$

From (2.49) we know that

$$[j]p_m(j) = (-1)^m B_m, \quad m \geq 2. \quad (4.17)$$

From (2.53) we get

$$m[j]q_m(j) = -B_m, \quad m \geq 2. \quad (4.18)$$

Replacing m by $2m$, we obtain

$$[j]q_{2m}(j) = -\frac{B_{2m}}{2m}, \quad m \geq 1. \quad (4.19)$$

Substituting (4.19) into (4.16) and (4.14), we complete the proof. □

Proposition 8. *For any $n \geq 2$,*

$$S_{2,0}(2n-1) = -\frac{3B_{2n}}{n}. \quad (4.20)$$

Proof. From Proposition 7 we know it suffices to show that

$$S_{2,0}(2n-1) + 3S_{1,0}(2n-1) = 0. \quad (4.21)$$

We observe that

$$[j^2]\left(x_2\mu\nu^2 + x_1\mu\nu\right) = [j^2]\left(x_2 j^2(j-1)^2(2j-1) + x_1 j(j-1)(2j-1)\right) = -x_2 - 3x_1.$$

Comparing the coefficients of j^2 on both sides of (4.15), we deduce that

$$\begin{aligned}
&-S_{2,0}(2n-1) - 3S_{1,0}(2n-1) \\
&= -2[j^2]q_{2n}(j) - \sum_{m=1}^{2n-1}(-1)^m[j]q_m(j)\cdot[j]q_{2n-m}(j) - \sum_{m=0}^{2n-1}S_{1,0}(m-1)[j]q_{2n-m}(j) \\
&= -2[j^2]q_{2n}(j) - \sum_{m=1}^{n-1}[j]q_{2m}(j)[j]q_{2n-2m}(j) - \sum_{m=1}^{n-1}S_{1,0}(2m-1)[j]q_{2n-2m}(j)
\end{aligned}$$

$$= -2[j^2]q_{2n}(j) + \sum_{m=1}^{n-1}[j]q_{2m}(j)\cdot[j]q_{2n-2m}(j), \tag{4.22}$$

where in the last equality we used (4.16). Hence the proposition is equivalent to the assertion that for any $n \geq 2$,

$$2[j^2]q_{2n}(j) = \sum_{m=1}^{n-1}[j]q_{2m}(j)\cdot[j]q_{2n-2m}(j). \tag{4.23}$$

From (2.49) we deduce that

$$[j^2]p_m(j) = \frac{(-1)^{m-1}}{2}mB_{m-1}.$$

Hence for $m \geq 2$,

$$[j^2]p_{2m}(j) = 0. \tag{4.24}$$

From (2.53) we deduce that for $n \geq 2$,

$$2n[j^2]q_{2n}(j) = -[j^2]p_{2n}(j) + \sum_{k=2}^{2n-1}(-1)^{k-1}[j]p_k(j)[j]q_{2n-k}(j).$$

Using (4.17), (4.19) and (4.24), we obtain

$$[j^2]q_{2n}(j) = \frac{1}{2n}\sum_{k=1}^{n-1}\frac{B_{2k}B_{2n-2k}}{2n-2k}. \tag{4.25}$$

From (4.19) we have

$$\begin{aligned}
&\sum_{m=1}^{n-1}[j]q_{2m}(j)\cdot[j]q_{2n-2m}(j)\\
=&\sum_{m=1}^{n-1}\frac{B_{2m}}{2m}\cdot\frac{B_{2n-2m}}{2n-2m}\\
=&\sum_{m=1}^{n-1}B_{2m}B_{2n-2m}\frac{1}{2n}\left(\frac{1}{2m}+\frac{1}{2n-2m}\right)\\
=&\frac{1}{n}\sum_{m=1}^{n-1}\frac{B_{2m}B_{2n-2m}}{2n-2m}.
\end{aligned} \tag{4.26}$$

Comparing (4.25) and (4.26), we complete the proof of (4.23) and the proposition. □

4.3. Alternative representations of C_n

The representations of C_n are not unique. Indeed, it is possible to represent C_n using only A_0, A_1 and A_2. For this we need to know the relation between A_3 and A_0, A_1, A_2. Recall that E_2, E_4 and E_6 denotes three Eisenstein series as given in (1.11)–(1.13). The following identities of Ramanujan are well-known (see e.g. [1, Theorem 4.2.3]):

$$\Theta(E_2) = \frac{E_2^2 - E_4}{12}, \tag{4.27}$$

$$\Theta(E_4) = \frac{E_2E_4 - E_6}{3}, \tag{4.28}$$

$$\Theta(E_6) = \frac{E_2E_6 - E_4^2}{2}. \tag{4.29}$$

We first express E_2, E_4 and E_6 in terms of A_0, A_1 and A_2.

Proposition 9. *We have*

$$E_2 = 1 - 24A_0, \tag{4.30}$$

$$E_4 = 1 - 48A_0 + 576A_0^2 + 288A_1, \tag{4.31}$$

$$E_6 = 1 - 72A_0 + 1728A_0^2 - 13824A_0^3 + 432A_1 - 10368A_0A_1 - 864A_2. \tag{4.32}$$

Proof. The relation (4.30) follows from definition.

Since $\Theta(A_0) = A_1$, (4.27) implies

$$E_4 = E_2^2 - 12\Theta(E_2) = E_2^2 + 288A_1 = 1 - 48A_0 + 576A_0^2 + 288A_1.$$

This proves (4.31).

Next, we have

$$\Theta(E_2^2) = \Theta(1 - 48A_0 + 576A_0^2) = -48A_1 + 1152A_0A_1. \tag{4.33}$$

Applying Θ to both sides of (4.27), by (4.28) and (4.33) we obtain

$$\begin{aligned}\Theta^2(E_2) &= \frac{1}{12}\Theta(E_2^2 - E_4) \\ &= \frac{1}{12}\Theta(E_2^2) - \frac{1}{36}(E_2E_4 - E_6) \\ &= 96A_0A_1 - 4A_1 - \frac{1}{36}(E_2E_4 - E_6).\end{aligned}$$

On the other hand, we have

$$\Theta^2(E_2) = -24\Theta^2(A_0) = -24A_2. \tag{4.34}$$

So we deduce that

$$A_2 = -4A_0A_1 + \frac{1}{6}A_1 + \frac{1}{864}(E_2E_4 - E_6). \tag{4.35}$$

This implies

$$E_6 = E_2E_4 - 3456A_0A_1 + 144A_1 - 864A_2. \tag{4.36}$$

Substituting (4.30) and (4.31) into (4.36) and simplifying, we obtain (4.32). □

From Proposition 9, it is easy to express A_0, A_1 and A_2 as polynomials in E_2, E_4 and E_6.

Corollary 2. *We have*

$$\begin{aligned} A_0 &= \frac{1}{24}(1 - E_2),\\ A_1 &= \frac{1}{288}(E_4 - E_2^2),\\ A_2 &= -\frac{1}{1728}(E_2^3 - 3E_2E_4 + 2E_6). \end{aligned}$$

Lemma 10. *For any $n \geq 1$, A_n can be written as a multivariate polynomial in A_0, A_1 and A_2 with integer coefficients and degree at most $n-1$. In particular, we have*

$$A_3 = A_2 + 36A_1^2 - 24A_0A_2. \tag{4.37}$$

Proof. Applying the Θ operator to both sides of (4.35), upon using (4.27)–(4.29) and simplifying, we obtain

$$\begin{aligned} A_3 &= -4\Theta(A_0A_1) + \frac{1}{6}\Theta(A_1) + \frac{1}{864}\Theta(E_2E_4 - E_6)\\ &= -4A_0A_2 - 4A_1^2 + \frac{1}{6}A_2 + \frac{1}{864}\left(\Theta(E_2)E_4 + E_2\Theta(E_4) - \Theta(E_6)\right)\\ &= -4A_0A_2 - 4A_1^2 + \frac{1}{6}A_2 + \frac{5}{10368}\left(E_2^2E_4 + E_4^2 - 2E_2E_6\right). \end{aligned}$$

Now substituting (4.30)–(4.32) into the above identity and simplifying, we obtain (4.37).

Since $A_{m+1} = \Theta(A_m)$, the first assertion follows by using (4.37) and induction on m. □

Finally, we present a proof of Theorem 2.

Proof of Theorem 2. From Lemma 10 and Proposition 5, we know that C_n can be represented as a polynomial of A_0, A_1 and A_2. For the uniqueness, it is known that E_2,

E_4 and E_6 are algebraically independent over $\mathbb{C}$ (see [16, Lemma 117], for example). Therefore, Corollary 2 implies that A_0, A_1 and A_2 are also algebraically independent over $\mathbb{C}$. Hence the expression of C_n as a polynomial in A_0, A_1 and A_2 is unique. From Theorem 1 and Lemma 10, it is easy to see that all the coefficients are rational numbers.

From Lemma 10, we see that $A_n = A_2 +$ higher degree terms for all $n \geq 3$. So Proposition 6 still holds for this representation of C_n in A_0, A_1 and A_2, and the coefficients of A_0 and A_1 do not change. Therefore, the coefficients of the linear terms A_0, A_1, A_2 in this representation of C_n are $6S_{1,0}(n)$, $12S_{2,0}(n)$, $(-1)^{n-1} - 6S_{1,0}(n) - 12S_{2,0}(n)$, respectively. Since $S_{1,0}(n)$ and $S_{2,0}(n)$ are given explicitly in Propositions 7 and 8, we complete our proof of Theorem 2. □

Acknowledgments

We are grateful to the referees for their careful reading of the manuscript and helpful comments. We would like to thank Professor Alan Sokal, whose questions stimulated this research, for his valuable comments on the preprint. The first author was supported by "the Fundamental Research Funds for the Central Universities" (Grant No. 1301–413000053) and a start-up research grant (No. 1301–413100048) of the Wuhan University.

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