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ON A CONJECTURE OF KIMOTO AND WAKAYAMA

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ABSTRACT. We prove a conjecture due to Kimoto and Wakayama from 2006 concerning Apéry-like numbers associated to a special value of a spectral zeta function. Our proof uses hypergeometric series and p -adic analysis.

1. INTRODUCTION

Let $Q = Q_{\alpha, \beta}$ be the ordinary differential operator on $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ defined by

$$Q := \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} \left(-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 \right) + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \left(x \frac{d}{dx} + \frac{1}{2} \right)$$

where α, β are positive real numbers satisfying $\alpha\beta > 1$. The system defined by the operator Q is called the *non-commutative harmonic oscillator* [8]. The operator Q is positive, self-adjoint and unbounded with a discrete spectrum in which the multiplicities of the eigenvalues

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \dots (\rightarrow \infty)$$

are uniformly bounded. Thus, one can define the *spectral zeta function*

$$\zeta_Q(s) := \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s}.$$

The series $\zeta_Q(s)$ is absolutely convergent, defines a holomorphic function in s for $\operatorname{Re}(s) > 1$ and can be meromorphically continued to \mathbb{C} (for details, see [2], [3]). In [4], Kimoto and Wakayama discuss the Apéry-like numbers

$$\tilde{J}_2(n) := \sum_{k=0}^n (-1)^k \binom{-\frac{1}{2}}{k}^2 \binom{n}{k}$$

which occur in a representation of the special value $\zeta_Q(2)$. Similar to the Apéry numbers for $\zeta(2)$ and $\zeta(3)$, these numbers satisfy the recurrence relation (see Proposition 4.11 in [3])

$$4n^2 \tilde{J}_2(n) - (8n^2 - 8n + 3) \tilde{J}_2(n-1) + 4(n-1)^2 \tilde{J}_2(n-2) = 0,$$

with $\tilde{J}_2(0) = 1$ and $\tilde{J}_2(1) = \frac{3}{4}$, possess many interesting arithmetic properties such as

$$\tilde{J}_2(mp^r) \equiv \tilde{J}_2(mp^{r-1}) \pmod{p^r}$$

for integers $m, r \geq 1$ and primes $p \geq 3$ (see Theorem 6.2 of [4]) and have the modular parametrization (see Theorem 5.1 in [5] or #19 in Zagier's list [11])

$$\frac{\eta(2z)^{22}}{\eta(z)^{12}\eta(4z)^8} = \sum_{n=0}^{\infty} \tilde{J}_2(n) t^n$$

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where

$$t = t(z) = 16 \frac{\eta(z)^8 \eta(4z)^{16}}{\eta^{24}(2z)}$$

and $\eta(z)$ is the Dedekind eta-function. Our interest concerns the following conjecture from [4].

Conjecture 1. (*Kimoto-Wakayama*) For primes $p \geq 3$,

$$\sum_{k=0}^{p-1} \tilde{J}_2(k)^2 \equiv (-1)^{\frac{p-1}{2}} \pmod{p^3}.$$

In this paper, we prove two results, the second of which is equivalent to Conjecture 1. Recall that for a nonnegative integer r and $\alpha_i, \beta_i \in \mathbb{C}$ with $\beta_i \notin \{\dots, -3, -2, -1\}$, the (generalized) hypergeometric series ${}_{r+1}F_r$ is defined by

$${}_{r+1}F_r \left[\begin{matrix} \alpha_1 & \alpha_2 & \dots & \alpha_{r+1} \\ \beta_1 & \dots & \beta_r \end{matrix} ; \lambda \right] := \sum_{k=0}^{\infty} \frac{(\alpha_1)_k (\alpha_2)_k \dots (\alpha_{r+1})_k}{(\beta_1)_k \dots (\beta_r)_k} \cdot \frac{\lambda^k}{k!},$$

where $(a)_0 := 1$ and $(a)_k := a(a+1)\dots(a+k-1)$. This series converges for $|\lambda| < 1$. Hypergeometric series are an important class of special functions which have been investigated by Gauss, Euler, and Kummer and have numerous applications to the theory of differential equations, algebraic varieties and physics. For a thorough treatment of hypergeometric series, the reader is referred to [1]. Note that

$$\tilde{J}_2(n) = {}_3F_2 \left[\begin{matrix} \frac{1}{2} & \frac{1}{2} & -n \\ 1 & 1 \end{matrix} ; 1 \right].$$

Theorem 2. For primes $p > 3$,

$$(1) \quad \sum_{x=0}^{p-1} {}_3F_2 \left[\begin{matrix} \frac{1-p}{2} & \frac{1+p}{2} & -x \\ 1 & 1 \end{matrix} ; 1 \right]^2 \equiv (-1)^{\frac{p-1}{2}} \pmod{p^3}$$

and for primes $p \geq 3$

$$(2) \quad \sum_{x=0}^{p-1} {}_3F_2 \left[\begin{matrix} \frac{1}{2} & \frac{1}{2} & -x \\ 1 & 1 \end{matrix} ; 1 \right]^2 \equiv (-1)^{\frac{p-1}{2}} \pmod{p^3}.$$

The proof of Theorem 2 uses hypergeometric series and p -adic analysis. The paper is organized as follows. In Section 2, we briefly recall the required background concerning hypergeometric series, then prove Theorem 2. Finally, we have numerically observed the following generalization of (2): for primes $p \geq 3$ and integers $r \geq 1$,

$$\sum_{x=0}^{p^r-1} {}_3F_2 \left[\begin{matrix} \frac{1}{2} & \frac{1}{2} & -x \\ 1 & 1 \end{matrix} ; 1 \right]^2 \equiv (-1)^{\frac{p-1}{2}} \sum_{x=0}^{p^{r-1}-1} {}_3F_2 \left[\begin{matrix} \frac{1}{2} & \frac{1}{2} & -x \\ 1 & 1 \end{matrix} ; 1 \right]^2 \pmod{p^{3r}}.$$

We leave this to the interested reader.

2. PROOF OF THEOREM 2

The proof below is motivated by the approach of Rutkowski in [9]. We start with some preliminaries.

2.1. Preliminaries.

Lemma 3. *Given integers j, k, m , with $m \geq 1$, and $j, k \geq 0$,*

$$\sum_{x=0}^{m-1} (x-j+1)_{j+k} = \frac{(m-j)_{j+k+1}}{j+k+1}.$$

Proof. First, we observe that the identity holds trivially when $m \leq j$ since both sides are 0. Thus we assume $m > j$. Moreover, the identity holds when $j = k = 0$ as both sides are m . We note that $(x)_{n+1} - (x-1)_{n+1} = (n+1)(x)_n$ holds for integers $x \geq 0$, $n \geq 1$. Then for any positive integer N ,

$$(N)_{n+1} = \sum_{x=0}^N ((x)_{n+1} - (x-1)_{n+1}) = (n+1) \sum_{x=0}^N (x)_n.$$

Letting $N = m - j$ and $n = j + k$ gives

$$\sum_{x=0}^{m-j} (x)_{j+k} = \frac{(m-j)_{j+k+1}}{j+k+1},$$

which is equivalent to

$$\sum_{x=j}^{m-1} (x-j+1)_{j+k} = \frac{(m-j)_{j+k+1}}{j+k+1}.$$

Since $(x-j+1)_{j+k} = 0$ for $0 \leq x < j$, this yields the lemma. \square

We now fix some notation for the duration of the paper. Since one can verify (2) directly for $p = 3$, we fix $p > 3$ prime and $n = \frac{p-1}{2}$. Given a function $g(x)$, we define (see [9])

$$I(g) = \sum_{x=0}^{p-1} g(x).$$

Let $f_n(x)$ be the degree n polynomial in $\mathbb{Z}_p[x]$ defined by

$$(3) \quad f_n(x) = \sum_{j=0}^n \binom{n}{j} \binom{n+j}{j} \binom{x}{j} = {}_3F_2 \left[\begin{matrix} -n & 1+n & -x \\ & 1 & 1 \end{matrix} ; 1 \right].$$

These are orthogonal polynomials satisfying the following recursion (see (4) of [10])

$$(n+1)^2 f_{n+1}(x) = (2n+1)(2x+1)f_n(x) + n^2 f_{n-1}(x).$$

Furthermore, let $g(x)$ be the degree $p-1$ polynomial in $\mathbb{Z}_p[x]$ defined by

$$(4) \quad g(x) = \sum_{j=0}^{p-1} (-1)^j \binom{-\frac{1}{2}}{j}^2 \binom{x}{j} = {}_3F_2 \left[\begin{matrix} \frac{1}{2} & \frac{1}{2} & -x \\ & 1 & 1 \end{matrix} ; 1 \right]_{p-1}$$

where the subscript in (4) denotes the truncation of the sum at $p-1$.

2.2. Relationship between (1) and (2). With our new notation, (1) is equivalent to

$$(5) \quad I(f_n(x)^2) \equiv (-1)^n \pmod{p^3},$$

while (2) is equivalent to

$$I(g(x)^2) \equiv (-1)^n \pmod{p^3}.$$

First, by (3) and (4), we observe that

$$g(x) - f_n(x) = \sum_{k=1}^n \frac{\left(\left(\frac{1}{2}\right)_k^2 - \left(\frac{1-p}{2}\right)_k \left(\frac{1+p}{2}\right)_k\right) (-x)_k}{k!^3} + \sum_{k=\frac{p+1}{2}}^{p-1} \frac{\left(\frac{1}{2}\right)_k^2 (-x)_k}{k!^3}.$$

Since $\left(\frac{1}{2}\right)_k^2 \equiv \left(\frac{1-p}{2}\right)_k \left(\frac{1+p}{2}\right)_k \pmod{p^2}$, and $\left(\frac{1}{2}\right)_k \equiv 0 \pmod{p}$ for $k \geq \frac{p+1}{2}$, we see that $g(x) - f_n(x) \in p^2 x \mathbb{Z}_p[x]$ of degree $p-1$. Thus, $g(x) = f_n(x) + p^2 h(x)$, where $h(x) \in x \mathbb{Z}_p[x]$ has degree $p-1$. This yields that

$$I(g(x)^2) \equiv I(f_n(x)^2) + 2p^2 I(f_n(x)h(x)) \pmod{p^3}.$$

Note that if we prove

$$(6) \quad I(f_n(x)g(x)) \equiv I(f_n(x)^2) \pmod{p^3},$$

then we can conclude $I(f_n(x)h(x)) \equiv 0 \pmod{p}$ and thus $I(g(x)^2) \equiv I(f_n(x)^2) \pmod{p^3}$. Hence, in order to prove Theorem 2, it suffices to prove (5) and (6).

2.3. Proof of Theorem 2. From (3) and (4), we have

$$(7) \quad I(f_n(x)^2) = \sum_{j=0}^n \binom{n}{j} \binom{n+j}{j} I\left(f_n(x) \cdot \binom{x}{j}\right),$$

$$(8) \quad I(f_n(x)g(x)) = \sum_{j=0}^{p-1} (-1)^j \binom{-\frac{1}{2}}{j}^2 I\left(f_n(x) \cdot \binom{x}{j}\right).$$

Note that $\binom{n}{j}$, $\binom{n+j}{j}$, and $j!$ do not introduce any factors of p ; $\binom{-\frac{1}{2}}{j}$ has no factors of p when $0 \leq j \leq n$, but does contain a copy of p when $n < j \leq p-1$. We also observe that

$$(9) \quad (-1)^j \binom{-\frac{1}{2}}{j}^2 \equiv \binom{n}{j} \binom{n+j}{j} \pmod{p^2},$$

so (6) is true modulo p^2 . For a finer analysis we study $I\left(f_n(x) \cdot \binom{x}{j}\right)$ modulo p^3 .

Lemma 4. For any $j \geq 0$, $m \geq 1$,

$$I\left(f_m(x) \cdot \binom{x}{j}\right) = (-1)^m \sum_{k=0}^m \binom{m}{k} \binom{m+k}{k} \frac{(-1)^k (p-j)_{j+k+1}}{j!k!(j+k+1)}.$$

Proof. We use the following identity (see page 142 of [1]). When m is a positive integer and both sides converge,

$$(10) \quad {}_3F_2 \left[\begin{matrix} -m & a & b \\ & d & e \end{matrix} ; 1 \right] = \frac{(e-a)_m}{(e)_m} {}_3F_2 \left[\begin{matrix} -m & a & d-b \\ & d & a+1-m-e \end{matrix} ; 1 \right].$$

Letting $a = 1 + m$, $b = -x$, $d = e = 1$ in (10) yields

$$f_m(x) = (-1)^m {}_3F_2 \left[\begin{matrix} -m & 1+m & 1+x \\ & 1 & 1 \end{matrix} ; 1 \right] = (-1)^m \sum_{k=0}^m \binom{m}{k} \binom{m+k}{k} \binom{-1-x}{k},$$

and thus

$$I\left(f_m(x) \cdot \binom{x}{j}\right) = (-1)^m \sum_{k=0}^m \binom{m}{k} \binom{m+k}{k} I\left(\binom{x}{j} \binom{-1-x}{k}\right).$$

Since $\binom{x}{j} \binom{-1-x}{k} = \frac{(-1)^k (x-j+1)_{j+k}}{j!k!}$, Lemma 3 yields the result. \square

From Lemma 4, we are now able to analyze $I\left(f_n(x) \cdot \binom{x}{j}\right)$ modulo p^3 . We will use the following identities from Rutkowski [9]. For $j = 0, 1, \dots, n-1$,

$$(11) \quad \sum_{k=0}^n \frac{(-1)^k}{j+k+1} \binom{n+k}{k} \binom{n}{k} = 0,$$

and for $j = n$

$$(12) \quad \sum_{k=0}^n \frac{(-1)^k}{n+k+1} \binom{n+k}{k} \binom{n}{k} = \frac{(-1)^n}{2n+1} \binom{2n}{n}^{-1}.$$

We note that these identities are direct consequences of the Pfaff-Saalschütz formula (Theorem 2.2.6 of [1]), which says that for $n \in \mathbb{N}$,

$$(13) \quad {}_3F_2 \left[\begin{matrix} -n & a & b \\ c & 1+a+b-c-n & \end{matrix}; 1 \right] = \frac{(c-a)_n (c-b)_n}{(c)_n (c-a-b)_n}.$$

Letting $a = n+1$, $b = j+1$, and $c = 1$ yields

$$\sum_{k=0}^n \frac{(-1)^k}{j+k+1} \binom{n+k}{k} \binom{n}{k} = \frac{1}{j+1} \cdot {}_3F_2 \left[\begin{matrix} -n & n+1 & j+1 \\ 1 & j+2 & \end{matrix}; 1 \right] = \frac{1}{j+1} \cdot \frac{(-n)_n (-j)_n}{(1)_n (-1-n-j)_n},$$

which gives (11) and (12).

Let $H_k = \sum_{j=1}^k \frac{1}{j}$ denote the k th harmonic number where $H_0 := 0$. Note that for $0 \leq k < p$, $H_k \in \mathbb{Z}_p$. The following lemma is the key for proving Theorem 2.

Lemma 5. *Let $p > 3$ be prime and $n = \frac{p-1}{2}$. For integers $0 \leq j \leq p-1$,*

$$(14) \quad \begin{aligned} I\left(f_n(x) \cdot \binom{x}{j}\right) &\equiv p(-1)^{n+j} \sum_{k=0}^n \frac{(-1)^k}{j+k+1} \binom{n}{k} \binom{n+k}{k} \\ &\quad + p^2(-1)^{n+j} \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \frac{(-1)^k [H_k - H_j]}{j+k+1} \pmod{p^2}. \end{aligned}$$

Moreover, when $0 \leq j < n$,

$$(15) \quad I\left(f_n(x) \cdot \binom{x}{j}\right) \equiv p^2(-1)^{n+j} \sum_{k=0}^n \frac{\binom{n}{k} \binom{n+k}{k} (-1)^k [H_k - H_j]}{j+k+1} \pmod{p^3},$$

and when $j = n$,

$$(16) \quad I\left(f_n(x) \cdot \binom{x}{n}\right) \equiv (-1)^n \binom{2n}{n}^{-1} + p^2 \sum_{k=0}^n \frac{\binom{n}{k} \binom{n+k}{k} (-1)^k [H_k - H_n]}{n+k+1} \pmod{p^3}.$$

Proof. We first observe that when $0 \leq k \leq n$ and $0 \leq j \leq p-1$, we have

$$(17) \quad \begin{aligned} \frac{(p-j)_{j+k+1}}{j!k!} &= \left(\frac{p}{j} - 1\right) \left(\frac{p}{j-1} - 1\right) \cdots \left(\frac{p}{1} - 1\right) p \left(\frac{p}{1} + 1\right) \cdots \left(\frac{p}{k} + 1\right) \\ &\equiv p(-1)^j (1 + p[H_k - H_j]) \pmod{p^3} \end{aligned}$$

and thus (14) follows from Lemma 4 with $m = n$ since $j+k+1$ introduces at most one factor of p in the denominator. Now, if $0 \leq j < n$, then $p \nmid j+k+1$ and so Lemma 4, (11), and (17) imply (15). We now note that letting $j = k = n$ in (17) gives

$$(18) \quad \frac{(p-n)_{2n+1}}{n!^2} \equiv p(-1)^n \pmod{p^3}.$$

Thus, after taking $m = n$ in Lemma 4, applying (18) to the $k = n$ term, then applying (17) with $j = n$ to the $0 \leq k < n$ terms and recombining, we have

$$\begin{aligned} I \left(f_n(x) \cdot \binom{x}{n} \right) &\equiv (-1)^n \sum_{k=0}^{n-1} \binom{n}{k} \binom{n+k}{k} \frac{(-1)^k (p-n)_{n+k+1}}{n!k!(n+k+1)} + (-1)^n \binom{2n}{n} \pmod{p^3} \\ &\equiv p \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \frac{(-1)^k}{n+k+1} + p^2 \sum_{k=0}^n \frac{\binom{n}{k} \binom{n+k}{k} (-1)^k [H_k - H_n]}{n+k+1} \pmod{p^3}. \end{aligned}$$

Using (12), we arrive at (16). \square

Finally, we need two additional lemmas. The first is from [7].

Lemma 6. *Let $p > 3$ be prime and $n = \frac{p-1}{2}$. We have*

$$\binom{-\frac{1}{2}}{n}^2 \equiv (-1)^n \binom{2n}{n} \pmod{p^3}.$$

Lemma 7. *Let $p > 3$ be prime and $n = \frac{p-1}{2}$. We have*

$$p \sum_{j=n+1}^{p-1} \binom{-\frac{1}{2}}{j}^2 \sum_{k=0}^n \frac{(-1)^k}{j+k+1} \binom{n}{k} \binom{n+k}{k} \equiv 0 \pmod{p^3}.$$

Proof. We note that if i is a fixed integer such that $1 \leq i \leq n$, then since $-n \equiv n+1 \pmod{p}$,

$$(19) \quad \begin{aligned} (n-i)!^2 &= (n-(n-1))^2 \cdots (n-j)^2 \cdots (n-i)^2 \\ &\equiv (p-1)^2 \cdots (n+1+j)^2 \cdots (1+n+i)^2 \pmod{p}. \end{aligned}$$

Thus $(n-i)!^2(n+i)!^2 \equiv 1 \pmod{p}$ by Wilson's theorem. Also

$$\binom{1}{2}_{n+i} = \binom{1}{2}_n \binom{p}{2} \binom{p}{2+1} \cdots \binom{p}{2+i-1} \equiv \frac{p}{2} \binom{1}{2}_n (i-1)! \pmod{p^2},$$

and thus

$$(20) \quad \binom{1}{2}_{n+i}^2 \equiv \frac{p^2}{4} \binom{1}{2}_n^2 (i-1)!^2 \pmod{p^3}.$$

Similarly,

$$(21) \quad \binom{1}{2}_n^2 = \binom{1}{2}_{n-i}^2 \binom{p}{2-1}^2 \cdots \binom{p}{2-i}^2 \equiv i!^2 \binom{1}{2}_{n-i}^2 \pmod{p}.$$

By (9), it suffices to prove

$$p \sum_{j=n+1}^{p-1} \sum_{k=0}^n \frac{\binom{1}{2}_j^2 \binom{1}{2}_k^2}{j!^2 k!^2} \cdot \frac{1}{j+k+1} \equiv 0 \pmod{p^3}.$$

Since $j \geq n+1$, we have $p^2 \mid \binom{1}{2}_j^2$ and thus the summand is 0 modulo p^3 when $j+k+1 \neq p$. Using (19)–(21), and the fact (see [6]) that $\sum_{i=1}^n \frac{1}{i^2} \equiv 0 \pmod{p}$, we have

$$\begin{aligned}
p \sum_{j=n+1}^{p-1} \sum_{k=0}^n \frac{\left(\frac{1}{2}\right)_j^2 \left(\frac{1}{2}\right)_k^2}{j!^2 k!^2} \cdot \frac{1}{j+k+1} &\equiv \sum_{j=n+1}^{p-1} \frac{\left(\frac{1}{2}\right)_j^2 \left(\frac{1}{2}\right)_{p-1-j}^2}{j!^2 (p-1-j)!^2} \pmod{p^3} \\
&= \sum_{i=1}^n \frac{\left(\frac{1}{2}\right)_{n+i}^2 \left(\frac{1}{2}\right)_{n-i}^2}{(n+i)!^2 (n-i)!^2} \\
&\equiv \frac{p^2}{4} \binom{1}{2}_n^4 \sum_{i=1}^n \frac{1}{i^2} \pmod{p^3} \\
&\equiv 0 \pmod{p^3}.
\end{aligned}$$

□

We now have the tools to prove Theorem 2.

Proof of Theorem 2. We first split (7) into the cases $j < n$ and $j = n$, and apply (15) and (16) to obtain

$$(22) \quad I(f_n(x)^2) \equiv (-1)^n + p^2 \cdot (-1)^n \sum_{j,k=0}^n \frac{\binom{n}{j} \binom{n+j}{j} \binom{n}{k} \binom{n+k}{k} (-1)^{k+j} [H_k - H_j]}{j+k+1} \pmod{p^3}.$$

As the sum on the right-hand side of (22) is symmetric in j and k , it equals 0 and thus (5) follows. We now split (8) into the cases when $j < n$, $j = n$, and $j > n$ to obtain $I(f_n(x)g(x)) = A + B + C$ where

$$\begin{aligned}
A &= \sum_{j=0}^{n-1} (-1)^j \binom{-\frac{1}{2}}{j}^2 I\left(f_n(x) \cdot \binom{x}{j}\right), \\
B &= (-1)^n \binom{-\frac{1}{2}}{n} I\left(f_n(x) \cdot \binom{x}{n}\right)
\end{aligned}$$

and

$$C = \sum_{j=n+1}^{p-1} (-1)^j \binom{-\frac{1}{2}}{j}^2 I\left(f_n(x) \cdot \binom{x}{j}\right).$$

When $0 \leq j < n$, we see from (15) that $I\left(f_n(x) \cdot \binom{x}{j}\right) \equiv 0 \pmod{p}$. Thus by (9) and Lemma 6 we have that

$$A + B \equiv I(f_n(x)^2) \pmod{p^3}.$$

Since p^2 divides $\binom{-\frac{1}{2}}{j}^2$ when $j > n$, applying (14) to C yields

$$\begin{aligned}
C &\equiv p \cdot (-1)^n \sum_{j=n+1}^{p-1} \binom{-\frac{1}{2}}{j}^2 \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \frac{(-1)^k}{j+k+1} \\
&\quad + p^2 \cdot (-1)^n \sum_{j=n+1}^{p-1} \binom{-\frac{1}{2}}{j}^2 \sum_{k=0}^n \binom{n}{k} \binom{n+k}{k} \frac{(-1)^k [H_k - H_j]}{j+k+1} \pmod{p^4}.
\end{aligned}$$

We observe that the first summand vanishes modulo p^3 by Lemma 7 and the second summand vanishes modulo p^3 since $j+k+1$ introduces at most one factor of p in the denominator. This proves (6). □

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