GAUSSIAN HYPERGEOMETRIC SERIES AND EXTENSIONS OF SUPERCONGRUENCES

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Abstract. Let p be an odd prime. The purpose of this paper is to refine methods of Ahlgren and Ono [2] and Kilbourn [13] in order to prove a general mod p^3 congruence for the Gaussian hypergeometric series ${}_{n+1}F_n(\lambda)$ where n is an odd positive integer. As a result, we extend three recent supercongruences. The first is a result of Ono and Ahlgren [2] on a supercongruence for Apéry numbers which was conjectured by Beukers in 1987. The second is one of Mortenson [18] which relates truncated hypergeometric series to the number of $\mathbb{F}_p$ points of some family of Calabi-Yau manifolds. Finally, the third is a result of Loh and Rhodes [16] on congruences between coefficients of modular forms corresponding to a particular class of elliptic curves and combinatorial objects. Additionally, we discuss the non-trivial methods of the computer summation package Sigma which were used to find explicit evaluations of two strange combinatorial identities involving generalized Harmonic sums.

1. Introduction

In the course of his work on proving the irrationality of $\zeta(3)$, Apéry introduced the following numbers. For a positive integer m, define

$$A(m) := \sum_{j=0}^{m} \binom{m+j}{j}^2 \binom{m}{j}^2.$$

These numbers are now known as the Apéry numbers. Several authors have subsequently studied many interesting congruence properties for $A(m)$ (see [5], [8], [17], [27]). In [4], Beukers was able to relate the Apéry numbers to the Fourier coefficients of a specific modular form. Namely, let

$$f(z) := \eta^4(2z)\eta^4(4z) = q\prod_{n=1}^{\infty}(1-q^{2n})^4(1-q^{4n})^4 = \sum_{n=1}^{\infty} a(n)q^n \tag{1}$$

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be the unique normalized eigenform in the space $S_4(\Gamma_0(8))$ of weight 4 cuspforms on $\Gamma_0(8)$. Here, as usual, $q := e^{2\pi iz}$ and

$$\eta(z) := q^{\frac{1}{24}} \prod_{n=1}^{\infty} (1 - q^n)$$

is the Dedekind eta function. Beukers proved that for all odd primes p, we have

$$A\Big(\frac{p-1}{2}\Big) \equiv a(p) \pmod{p}.$$

He then conjectured that the same congruence holds modulo p^2. This conjecture was proved for primes p such that $p \nmid a(p)$ by Ishikawa [12]. In [2], Ahlgren and Ono prove the conjecture unconditionally, namely

Theorem 1.1. [2] *Let p be an odd prime. Then*

$$A\Big(\frac{p-1}{2}\Big) \equiv a(p) \pmod{p^2}.$$

The idea of Theorem 1.1 is as follows. The authors first show that $a(p)$ can be expressed as a special value of the Gaussian hypergeometric function ${}_4F_3(\lambda)$ (see Section 2 for the definition of ${}_{n+1}F_n(\lambda)$). These functions are defined in terms of Jacobi sums. It is well known that Jacobi sums can be written in terms of Gauss sums. One then applies the Gross-Koblitz formula [11] to express the Gauss sums in terms of the p-adic Gamma function. Using combinatorial properties of the p-adic Gamma function combined with non-trivial Harmonic sum identities, Theorem 1.1 then follows. For an introduction to these methods, please see the monograph [23]. This general framework has been the basis for several recent results on supercongruences (see [1], [13], [16], [18], [19], [20]). The purpose of this paper is to refine the techniques of Ahlgren and Ono [2] and Kilbourn [13] in order to extend three supercongruences to higher powers of p.

Our first result extends Theorem 1.1 as follows.

Theorem 1.2. *Let p be an odd prime. For $x \in \mathbb{Z}_p$, let $G_1(x)$ and $G_2(x)$ be defined by (3) and (4) in Section 2. Then*

$$A\Big(\frac{p-1}{2}\Big) \equiv a(p) + \frac{p^2}{2} \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}^2 \binom{\frac{p-1}{2}}{j}^2 \Big(G_1(\tfrac{1}{2}+j) - G_2(\tfrac{1}{2}+j)\Big) \pmod{p^3}.$$

It is natural to wonder if there are congruences similar to Theorem 1.2 between Fourier coefficients of other modular forms and sums of products of binomial coefficients. In [29], Rodriguez-Villegas studied hypergeometric weight systems and numerically observed a number of congruences which relate truncated hypergeometric series to the number of $\mathbb{F}_p$ points of some family of Calabi-Yau manifolds. A hypergeometric weight system is a formal linear combination

$$\gamma = \sum_{k=1}^{\infty} \gamma_k [k],$$

where $\gamma_k \in \mathbb{Z}$ are zero for all but finitely many k, and for which the following two conditions are satisfied:

$$\sum_{k=1}^{\infty} k\gamma_k = 0,$$

$$d = d(\gamma) := -\sum_{k=1}^{\infty} \gamma_k > 0.$$

The positive integer d is called the dimension of γ. For a given γ, we associate a hypergeometric function

$$u(\lambda) := \sum_{n=0}^{\infty} u_n \lambda^n$$

where

$$u_n = \prod_{k=1}^{\infty} (kn)!^{\gamma_k}.$$

One can verify that for some minimal r, $u(\lambda)$ is related to an ordinary hypergeometric function, precisely

$$u(\lambda) = {}_rF_{r-1} \left(\begin{matrix} \alpha_1, & \ldots, & \alpha_r \\ \beta_1, & \ldots, & \beta_r \end{matrix} \mid \frac{\lambda}{\lambda_0} \right),$$

where

$$\lambda_0^{-1} := \prod_{k=1}^{\infty} k^{k\gamma_k}.$$

Here $0 \le \alpha_1 \le \alpha_2 \le \cdots \le \alpha_r < 1$ and $0 \le \beta_1 \le \beta_2 \le \cdots \le \beta_r < 1$ are two sets of r rational numbers. The numbers $\lambda_0 = \lambda_0(\gamma)$ and $r = r(\gamma)$ are called the special point and rank of γ, respectively.

The goal of [29] is to consider γ for which the truncation of $u(\lambda)$

$$\sum_{n=0}^{p-1} u_n \lambda^n \pmod{p}$$

is related to the number of points over $\mathbb{F}_p$ of some family of varieties X_λ. Rodriguez-Villegas shows that in the case where $d = r$, the coefficients u_n are integers for all n and thus the above truncation is well-defined. He then describes all cases with $d = r \leq 4$. It turns out that there are 14 values of γ with $d = r = 4$ and for each such γ one can associate a family of Calabi-Yau threefolds using toric geometry (for more details concerning this association see Sections 5 and 6 in [3]). At the special point $\lambda = \lambda_0$, Rodriguez-Villegas numerically observed that

$$\sum_{n=0}^{p-1} u_n \lambda_0^n \equiv c(p) \pmod{p^3}$$

for primes p not dividing λ_0^{-1}, where the $c(p)$ are Fourier coefficients of a weight four modular form which depends on γ. Of these 14 possible supercongruences, only one has been proven. Namely, if $\gamma = 4[2] - 8[1]$, then $\lambda_0 = 2^{-8}$, the modular form is (1), and Kilbourn [13] has proven the supercongruence

$$\sum_{n=0}^{p-1} \binom{2n}{n}^4 2^{-8n} \equiv a(p) \pmod{p^3}. \tag{2}$$

In future work, we plan to investigate the remaining 13 supercongruences in the case $d = r = 4$. What is also interesting is that supercongruences of a similar type hold for other dimensions. For $d = r = 2$, there are four values of γ and each value can be associated to a family of elliptic curves. In particular, for $\gamma = 2[2] - 4[1]$, Rodriguez-Villegas conjectured and Mortenson [18] proved the following supercongruence.

Theorem 1.3. [18] *If p is an odd prime, then*

$$\sum_{n=0}^{p-1} \binom{2n}{n}^2 16^{-n} \equiv \left(\frac{-4}{p}\right) \pmod{p^2}.$$

The second purpose of this paper is to extend Theorem 1.3 to a congruence mod p^3. Our result is the following.

Theorem 1.4. *Let p be an odd prime and let $\phi_p(\,\cdot\,)$ denote the Legendre symbol $\left(\frac{\cdot}{p}\right)$. Define*

$$C(p) := \frac{3}{32}\phi_p(-1)\left[\frac{1}{2} + \sum_{i=1}^{\frac{p-5}{2}} \frac{i!^2}{(2+2i)!}\right] + \frac{5}{8} + \frac{1}{16}\phi_p(-1)\sum_{i=1}^{\frac{p-1}{2}} \frac{(-1)^i}{i^2},$$

$$E(p) := p + \frac{3}{8}\phi_p(-1)\sum_{i=1}^{\frac{p-1}{2}} \binom{2i}{i}\frac{1}{i},$$

and

$$D(p) := \sum_{j=0}^{\frac{p-5}{2}} \frac{j!^2}{\prod_{i=0}^{j}(i+\frac{1}{2})^2}(j+1)^2.$$

Then

$$\sum_{n=0}^{\frac{p-1}{2}} \binom{2n}{n}^2 16^{-n} + p^2\Big[C(p)+D(p)\Big] + pE(p) \equiv \left(\frac{-4}{p}\right) \pmod{p^3}.$$

Since $p^2 \mid \binom{2n}{n}^2$ for all n with $\frac{p-1}{2} < n < p$ and $p \mid \sum_{i=1}^{\frac{p-1}{2}} \binom{2i}{i}\frac{1}{i}$, we recover Theorem 1.3 upon reducing mod p^2. We would like to point out that the remaining three mod p^2 supercongruences in the case $d = r = 2$ have been settled by Mortenson [19]. Also, a similar argument as in the proof of Theorem 1.4 in combination with Theorems 1 and 2 from [19] yields a mod p^3 extension to these three remaining cases. We do not discuss these extensions here.

Finally, consider the family of Legendre elliptic curves

$${}_2E_1(\lambda) : y^2 = x(x-1)(x-\lambda),$$

where $\lambda \in \mathbb{Q} \setminus \{0,1\}$. If p is an odd prime such that $p \nmid \lambda(\lambda-1)$, then p is a prime of good reduction for ${}_2E_1(\lambda)$. We define

$${}_2a_1(p;\lambda) := p + 1 - |{}_2E_1(\lambda)_p|,$$

where $|{}_2E_1(\lambda)_p|$ denotes the number of $\mathbb{F}_p$-points of ${}_2E_1(\lambda)_p$ including the point at infinity. It follows from a result of Diamond and Kramer [7] (and more generally [32]) that ${}_2a_1(p;\lambda)$ is the p-th coefficient of a modular form indexed by λ. Recently, Loh and Rhodes [16] proved the following supercongruence for ${}_2a_1(p;\lambda)$. For i, $n \in \mathbb{N}$, we define generalized Harmonic sums $H_n^{(i)}$ as

$$H_n^{(i)} := \sum_{j=1}^{n} \frac{1}{j^i}.$$

Theorem 1.5. [16] *If $\lambda \in \mathbb{Q} \setminus \{0,1\}$ and p is an odd prime for which $p \nmid \lambda(\lambda-1)$, then*

$${}_2a_1(p;\lambda)$$
$$\equiv \phi_p(-1)(p+1)\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}(-\lambda)^{jp}\Big(1+2jp(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j)\Big) \pmod{p^2}.$$

Our third result is an extension of Theorem 1.5 and states the following.

Theorem 1.6. *If $\lambda \in \mathbb{Q}\setminus\{0,1\}$ and p is an odd prime for which $p \nmid \lambda(\lambda-1)$, then*

$$
\begin{aligned}
&{}_2a_1(p;\lambda)\\
&\equiv p^2\phi_p(-1)\sum_{j=0}^{\frac{p-1}{2}}\binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}(-\lambda)^j\Bigg(1+4j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)\\
&\qquad\qquad+j^2\Big(2\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)^2-\Big(H^{(2)}_{\frac{p-1}{2}+j}-H^{(2)}_j\Big)\Big)\Bigg)\\
&+p\phi_p(-1)\sum_{j=0}^{\frac{p-1}{2}}\binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}(-\lambda)^{jp}\Bigg(1+j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)\\
&\qquad\qquad+j\Big(H^{(1)}_{\frac{p-1}{2}-j}-H^{(1)}_j\Big)\Bigg)\\
&+\phi_p(-1)\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j}\lambda^{jp^2}\\
&+p^2\phi_p(-1)\sum_{j=0}^{\frac{p-5}{2}}\frac{j!^2}{\prod_{i=0}^{j}(i+\frac{1}{2})^2}(j+1)^2\lambda^{j+1} \pmod{p^3}.
\end{aligned}
$$

Reductions of equation (14) mod p and equation (15) mod p^2 (see Section 3) and an application of Lemma 2.6 in conjunction with Theorem 3.2 and (27) imply Theorem 1.5.

Although Theorems 1.2, 1.4, and 1.6 do not hold mod p^4, one can still carry out the necessary, yet involved computations to determine $\left(\frac{-4}{p}\right)$, ${}_2a_1(p;\lambda)$ and $a(p)$ modulo p^4.

The paper is organized as follows. In Section 2, we recall Gaussian hypergeometric functions over finite fields and study properties of the p-adic Gamma function. In Section 3, we prove a general mod p^3 congruence for the Gaussian hypergeometric function ${}_{n+1}F_n(\lambda)$ for n odd (see Theorem 3.2). This congruence generalizes Theorem 2.4 in [16] and is the key result from which Theorems 1.2, 1.4, and 1.6 follow. In Section 4, we prove Theorems 1.2, 1.4, and 1.6 using the properties discussed in Section 2, Theorem 3.2, and two strange combinatorial identities which were discovered using computer summation program Sigma [30]. We note that the methods of

Section 4 in [13] (in particular defining an operator analogous to (4.12) in that paper) do not apply in our situation and thus we must appeal to computational methods (see Remark 4.1) to obtain Theorem 1.4. A description of the non-trivial methods involved using the Sigma package is included in Section 5. We should also mention that similar harmonic number identities were discovered and proven in [25].

2. Preliminaries

Greene [9], [10] defined hypergeometric functions over finite fields and showed that some of their properties are similar to ordinary hypergeometric functions. Let p be an odd prime and let $\mathbb{F}_p$ denote the finite field with p elements. We extend all characters χ of $\mathbb{F}_p^*$ to $\mathbb{F}_p$ by setting $\chi(0) := 0$. Following Greene, we give two definitions. The first definition is the finite field analogue of the binomial coefficient.

Definition 2.1. If A and B are characters of $\mathbb{F}_p$, then

$$\binom{A}{B} := \frac{B(-1)}{p} J(A, \bar{B}) = \frac{B(-1)}{p} \sum_{x \in \mathbb{F}_p} A(x)\bar{B}(1-x),$$

where $J(\chi, \psi)$ denotes the Jacobi sum if χ and ψ are characters of $\mathbb{F}_p$.

The second definition is the finite field analogue of ordinary hypergeometric functions.

Definition 2.2. If $A_0, A_1, \ldots, A_n$, and $B_1, \ldots, B_n$ are characters of $\mathbb{F}_p$, then the hypergeometric function ${}_{n+1}F_n\left(\begin{matrix} A_0, & A_1, & \ldots, & A_n \\ & B_1, & \ldots, & B_n \end{matrix} \mid x\right)_p$ is defined by

$${}_{n+1}F_n\left(\begin{matrix} A_0, & A_1, & \ldots, & A_n \\ & B_1, & \ldots, & B_n \end{matrix} \mid x\right)_p := \frac{p}{p-1} \sum_{\chi} \binom{A_0\chi}{\chi}\binom{A_1\chi}{B_1\chi} \cdots \binom{A_n\chi}{B_n\chi}\chi(x),$$

where the summation is over all characters χ of $\mathbb{F}_p$.

We restrict our attention to the case $A_i = \phi_p$ for all i and $B_j = \epsilon_p$ for all j where ϕ_p is the quadratic character and ϵ_p is the trivial character mod p. We shall denote this value by ${}_{n+1}F_n(\lambda)$. From Section 3 in [9], we have the following expression which relates a special value of ${}_2F_1(\lambda)$ to $\phi_p(-1)$.

Proposition 2.3. *If p is an odd prime, then*

$$p \cdot {}_2F_1(1) = -\phi_p(-1).$$

We also would like to recall the definition of the p-adic Gamma function and list some of its main properties. For more details, please consult [14],

[21], or [28]. Let $|\cdot|$ denote the p-adic absolute value on $\mathbb{Q}_p$. For $n \in \mathbb{N}$, we define

$$\Gamma_p(n) := (-1)^n \prod_{\substack{j<n \\ (j,p)=1}} j.$$

One can extend this function to all $x \in \mathbb{Z}_p$ upon setting

$$\Gamma_p(x) := \lim_{n \to x} \Gamma_p(n).$$

The following Proposition provides some of the main properties of Γ_p.

Proposition 2.4. *Let $n \in \mathbb{N}$ and $x \in \mathbb{Z}_p$. Then*

(1) $\Gamma_p(0) = 1$.
(2) $\dfrac{\Gamma_p(x+1)}{\Gamma_p(x)} = \begin{cases} -x & \text{if } |x| = 1, \\ -1 & \text{if } |x| < 1. \end{cases}$
(3) *If $0 \leq n \leq p-1$, then $n! = (-1)^{n+1}\Gamma_p(n+1)$.*
(4) $|\Gamma_p(x)| = 1$.
(5) *Let $x_0 \in [1, 2, \ldots, p]$ be the constant term in the p-adic expansion of x. Then $\Gamma_p(x)\Gamma_p(1-x) = (-1)^{x_0}$.*
(6) *If $x \equiv y \pmod{p^n}$, then $\Gamma_p(x) \equiv \Gamma_p(y) \pmod{p^n}$.*

For $x \in \mathbb{Z}_p$, we define

$$G_1(x) := \frac{\Gamma_p'(x)}{\Gamma_p(x)} \tag{3}$$

and

$$G_2(x) := \frac{\Gamma_p''(x)}{\Gamma_p(x)}. \tag{4}$$

One can check that $G_1(x)$ and $G_2(x)$ are defined for all $x \in \mathbb{Z}_p$ using the fact that $\Gamma_p(x)$ is locally analytic and $|\Gamma_p(x)| = 1$. We now mention some congruence properties of the p-adic Gamma function. For a proof of this result, see [6] or [13].

Proposition 2.5. *Let $p \geq 7$ be prime, $x \in \mathbb{Z}_p$, and $z \in p\mathbb{Z}_p$. Then*

(1) $G_1(x), G_2(x) \in \mathbb{Z}_p$.
(2) *We have*

$$\Gamma_p(x+z) \equiv \Gamma_p(x)\left(1 + zG_1(x) + \frac{z^2}{2}G_2(x)\right) \pmod{p^3}.$$

(3) $\Gamma_p'(x+z) \equiv \Gamma_p'(x) + z\Gamma_p''(x) \pmod{p^2}$.

Finally, we need the following combinatorial congruence which relates Γ_p to certain binomial coefficients.

Lemma 2.6. *If p is an odd prime and $1 \leq j \leq \frac{p-1}{2}$, then*

$$-\phi_p(-1)(-1)^j \binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j} \equiv \frac{\Gamma_p(\frac{1}{2}+j)^2}{\Gamma_p(1+j)^2} \pmod{p^2}.$$

Proof. By Proposition 2.4 (3) and (5), we have

$$\begin{aligned}
-\phi_p(-1)(-1)^j \binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j} &= -\phi_p(-1)(-1)^j \frac{(\frac{p-1}{2}+j)!}{j!^2(\frac{p-1}{2}-j)!} \\
&= \frac{\Gamma_p(\frac{1}{2}+j+\frac{p}{2})\Gamma_p(\frac{1}{2}+j-\frac{1}{2})}{\Gamma_p(1+j)^2}.
\end{aligned}$$

Now, using Proposition 2.5 (2), we have

$$\begin{aligned}
&\Gamma_p\Big(\frac{1}{2}+j+\frac{p}{2}\Big)\Gamma_p\Big(\frac{1}{2}+j-\frac{p}{2}\Big) \\
&\equiv \Big\{\Gamma_p\Big(\frac{1}{2}+j\Big)+\frac{p}{2}\Gamma_p'\Big(\frac{1}{2}+j\Big)\Big\}\Big\{\Gamma_p\Big(\frac{1}{2}+j\Big)-\frac{p}{2}\Gamma_p'\Big(\frac{1}{2}+j\Big)\Big\} \pmod{p^2} \\
&\equiv \Gamma_p\Big(\frac{1}{2}+j\Big)^2 \pmod{p^2}
\end{aligned}$$

and the result follows. □

3. A congruence for ${}_{n+1}F_n(\lambda)$

In this section, we prove a general mod p^3 congruence for ${}_{n+1}F_n(\lambda)$. We first need to define

$$A(j) := G_1(\tfrac{1}{2}+j) - G_1(1+j) \tag{5}$$

and for an odd positive integer n

$$\begin{aligned}
B(n,j) :=& \tfrac{n+1}{2}\Big(G_2(\tfrac{1}{2}+j)-G_2(1+j)\Big) + \tfrac{(n+1)n}{2}G_1(\tfrac{1}{2}+j)^2 \\
&+ \tfrac{(n+1)(n+2)}{2}G_1(1+j)^2 - (n+1)^2G_1(\tfrac{1}{2}+j)G_1(1+j).
\end{aligned} \tag{6}$$

We now require the following Lemma which relates $A(j)$ and $B(n,j)$ to generalized Harmonic sums.

Lemma 3.1. *Let p be an odd prime and $0 \leq j \leq \frac{p-1}{2}$. Let $A(j)$ and $B(n,j)$ be defined as in (5) and (6). Then*

$$A(j) \equiv H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j + 2p \sum_{r=0}^{j-1} \frac{1}{(2r+1)^2} \pmod{p^2} \tag{7}$$

and

$$B(n,j) \equiv \tfrac{(n+1)^2}{2} \Big(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j \Big)^2 - (\tfrac{n+1}{2}) \Big(H^{(2)}_{\frac{p-1}{2}+j} - H^{(2)}_j \Big) \pmod{p}. \tag{8}$$

Proof. For the proof of (7), see Lemma 4.1 in [13]. We now consider the proof of (8). Using Proposition 2.2 in [13] and Proposition 2.5 one can check that

$$G_2(\tfrac{1}{2}+j) - G_2(1+j) \equiv G_1(\tfrac{1}{2}+j)^2 - G_1(1+j)^2 - \Big(H^{(2)}_{\frac{p-1}{2}+j} - H^{(2)}_j \Big) \pmod{p}. \tag{9}$$

By (5), we have

$$A(j)^2 = G_1(\tfrac{1}{2}+j)^2 - G_1(1+j)^2 - 2G_1(\tfrac{1}{2}+j)G_1(1+j) + 2G_1(1+j)^2.$$

Thus by the definition of $B(n,j)$, (7), and (9), we have

$$\begin{aligned} B(n,j) &\equiv \tfrac{(n+1)^2}{2} A(j)^2 - (\tfrac{n+1}{2}) \Big(H^{(2)}_{\frac{p-1}{2}+j} - H^{(2)}_j \Big) \pmod{p} \\ &\equiv \tfrac{(n+1)^2}{2} \Big(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j \Big)^2 - (\tfrac{n+1}{2}) \Big(H^{(2)}_{\frac{p-1}{2}+j} - H^{(2)}_j \Big) \pmod{p}. \end{aligned}$$

□

We are now in a position to prove the key result from which Theorems 1.2, 1.4, and 1.6 will follow.

Theorem 3.2. *Let n be an odd positive integer, $l = \frac{n+1}{2}$, p be an odd prime, and define*

$$X(p,\lambda,n) := \phi_p(\lambda)\sum_{j=0}^{\frac{p-1}{2}}\binom{\frac{p-1}{2}+j}{j}^l\binom{\frac{p-1}{2}}{j}^l(-1)^{jl}\lambda^{-j}\Bigg(1+2(n+1)j\Big(H^{(1)}_{\frac{p-1}{2}+j}$$
$$-H^{(1)}_j\Big)+j^2\Big(\tfrac{n+1}{2}(1+n)\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)^2-(\tfrac{n+1}{2})\Big(H^{(2)}_{\frac{p-1}{2}+j}-H^{(2)}_j\Big)\Big)\Bigg),$$

$$Y(p,\lambda,n) := \phi_p(\lambda)\sum_{j=0}^{\frac{p-1}{2}}\binom{\frac{p-1}{2}+j}{j}^l\binom{\frac{p-1}{2}}{j}^l(-1)^{jl}\lambda^{-jp}\Bigg(1+(n+1)j\Big(H^{(1)}_{\frac{p-1}{2}+j}$$
$$-H^{(1)}_j\Big)-(\tfrac{n+1}{2})j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_{\frac{p-1}{2}-j}\Big)\Bigg),$$

$$Z(p,\lambda,n) := \phi_p(\lambda)(-\phi_p(-1))^l\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^{2l}16^{-jl}\lambda^{-jp^2},$$

and

$$D(p,\lambda) := \sum_{j=0}^{\frac{p-5}{2}}\frac{j!^2}{\prod_{i=0}^{j}(i+\frac{1}{2})^2}(j+1)^2\lambda^{-j-1}.$$

If $n\geq 3$*, then*

$$-p^n{}_{n+1}F_n(\lambda)\equiv p^2X(p,\lambda,n)+pY(p,\lambda,n)+Z(p,\lambda,n)\pmod{p^3}$$

and if $n=1$*, then*

$$-p_2F_1(\lambda)\equiv p^2\Big[X(p,\lambda,1)+D(p,\lambda)\Big]+pY(p,\lambda,1)+Z(p,\lambda,1)\pmod{p^3}.$$

Proof. Our starting point is an expression for $-p^n{}_{n+1}F_n(\lambda)$ which appears in [16]. Precisely, from page 316 of [16], we know that

$$-p^n{}_{n+1}F_n(\lambda)=\frac{1}{1-p}\sum_{\chi}J(\phi,\chi)^{n+1}\bar{\chi}(\lambda)$$

where $\bar{\chi}$ is the complex conjugate of χ. After expressing the Jacobi sum $J(\phi,\chi)^{n+1}$ in terms of Gauss sums, we then apply the Gross-Koblitz formula [11] to get (see [2], [16], or [18] for further details)

(10)

$$-p^n{}_{n+1}F_n(\lambda) = \frac{1}{1-p}\Bigg\{\phi_p(\lambda)+(-\phi_p(-1))^{\frac{n+1}{2}}\Bigg(\sum_{j=0}^{\frac{p-3}{2}} \frac{\Gamma_p(\frac{j}{p-1})^{n+1}}{\Gamma_p(\frac{1}{2}+\frac{j}{p-1})^{n+1}}\omega^j(\lambda) + p^{n+1}\sum_{j=\frac{p+1}{2}}^{p-2} \frac{\Gamma_p(\frac{j}{p-1})^{n+1}}{\Gamma_p(\frac{j}{p-1}-\frac{1}{2})^{n+1}}\omega^j(\lambda)\Bigg)\Bigg\}.$$

Here ω is the Teichmüller character which satisfies $\omega(\lambda) \equiv \lambda^{p^{s-1}} \pmod{p^s}$ and thus $\omega^j(\lambda) \equiv \lambda^{jp^{s-1}} \pmod{p^s}$ for $s \geq 1$. Assume that $n \geq 3$ is odd and thus the second sum in (10) vanishes modulo p^3. As $\frac{1}{1-p} \equiv 1+p+p^2 \pmod{p^3}$ and thus $\frac{j}{p-1} \equiv -j-jp-jp^2 \pmod{p^3}$, we apply parts (5) and (6) of Proposition 2.4 and reindex the summation to obtain

(11)

$$\begin{aligned} &-p^n{}_{n+1}F_n(\lambda)\\ &\equiv (1+p+p^2)\Bigg\{\phi_p(\lambda)\\ &+(-\phi_p(-1))^{\frac{n+1}{2}}\sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j+jp+jp^2)^{n+1}}{\Gamma_p(1+j+jp+jp^2)^{n+1}}\omega^{\frac{p-1}{2}-j}(\lambda)\Bigg\} \pmod{p^3}. \end{aligned}$$

By Proposition 2.5 (2), we see that

$$\begin{aligned} &\Gamma_p(x_0+j+jp+jp^2)^{n+1}\\ &\equiv \Gamma_p(x_0+j)^{n+1}\Big[1+(n+1)(jp+jp^2)G_1(x_0+j)\\ &+\tfrac{n+1}{2}(jp+jp^2)^2\Big(G_2(x_0+j)+nG_1(x_0+j)^2\Big)\Big] \pmod{p^3} \end{aligned}$$

for $x_0 \in \mathbb{Z}_p$. We expand the numerator and denominator of (11) with $x_0 = \frac{1}{2}$ and $x_0 = 1$ respectively. After multiplying the numerator and denominator by

$$1-(n+1)jpG_1(1+j)-\tfrac{n+1}{2}j^2p^2\Big(G_2(1+j)-(n+2)G_1(1+j)^2\Big)-(n+1)jp^2G_1(1+j),$$

we get

(12)
$$-p^n{}_{n+1}F_n(\lambda)$$
$$\equiv (1+p+p^2)\Bigg\{\phi_p(\lambda)+(-\phi_p(-1))^{\frac{n+1}{2}}\sum_{j=1}^{\frac{p-1}{2}}\frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}}\Big(1+(n+1)jpA(j)$$
$$+(n+1)jp^2A(j)+j^2p^2B(n,j)\Big)\omega^{\frac{p-1}{2}-j}(\lambda)\Bigg\} \pmod{p^3}$$

where $A(j)$ and $B(n,j)$ are defined by (5) and (6). We now need to consider the sums

(13)
$$\phi_p(\lambda)+(-\phi_p(-1))^{\frac{n+1}{2}}\sum_{j=1}^{\frac{p-1}{2}}\frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}}\Big(1+2(n+1)jA(j)+j^2B(n,j)\Big)\omega^{\frac{p-1}{2}-j}(\lambda),$$

$$\phi_p(\lambda)+(-\phi_p(-1))^{\frac{n+1}{2}}\sum_{j=1}^{\frac{p-1}{2}}\frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}}\Big(1+(n+1)jA(j)\Big)\omega^{\frac{p-1}{2}-j}(\lambda), \tag{14}$$

and

$$\phi_p(\lambda)+(-\phi_p(-1))^{\frac{n+1}{2}}\sum_{j=1}^{\frac{p-1}{2}}\frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}}\omega^{\frac{p-1}{2}-j}(\lambda) \tag{15}$$

which are the coefficients of p^2, p, and 1 respectively in (12). Observe that as we want to determine ${}_{n+1}F_n(\lambda)$ mod p^3, it suffices to compute (13) mod p, (14) mod p^2, and (15) mod p^3. Also note that

$$\omega^{\frac{p-1}{2}-j}(\lambda)=\omega^{\frac{p-1}{2}}(\lambda)\omega^{-j}(\lambda)=\phi_p(\lambda)\omega^{-j}(\lambda) \tag{16}$$

as ω is of order $p-1$. By Lemma 4.4 in [13], we see that

$$(\tfrac{n+1}{2})j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_{\frac{p-1}{2}-j}\Big)\equiv -2(n+1)jp\sum_{r=0}^{j-1}\frac{1}{(2r+1)^2} \pmod{p^2}. \tag{17}$$

By Lemma 2.6, we have

$$\left[-\phi_p(-1)(-1)^j\binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}\right]^{\frac{n+1}{2}} \equiv \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \pmod{p^2} \tag{18}$$

and so after combining Lemma 3.1, (16), (17), (18) and accounting for $j=0$, then (13) and (14) become $X(p,\lambda,n)$ and $Y(p,\lambda,n)$ respectively. Here we have used the fact that $\Gamma_p(1)^2 = 1$ and $\Gamma_p(\frac{1}{2})^2 = -\phi_p(-1)$ and thus for $n \geq 3$ odd

$$\frac{\Gamma_p(\frac{1}{2})^{n+1}}{\Gamma_p(1)^{n+1}} = 1.$$

By Proposition 2.5 in [18], we have

$$\frac{\Gamma_p(\frac{1}{2}+j)^2}{\Gamma_p(1+j)^2} = -\phi_p(-1)\binom{2j}{j}^2 16^{-j}$$

and thus using (16), we actually have equality between (15) and $Z(p,\lambda,n)$, namely

(19)

$$\phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \omega^{\frac{p-1}{2}-j}(\lambda)$$
$$= \phi_p(\lambda)(-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^{n+1} 16^{-j\left(\frac{n+1}{2}\right)} \lambda^{-jp^2}.$$

This proves the result for $n \geq 3$ odd. We now turn to the case $n=1$. By (10), we need only consider the last sum

$$-\phi_p(-1)p^2 \sum_{j=\frac{p+1}{2}}^{p-2} \frac{\Gamma_p(\frac{j}{p-1})^2}{\Gamma_p(\frac{j}{p-1}-\frac{1}{2})^2} \omega^j(\lambda).$$

By (5) and (6) of Proposition 2.4, we get

$$-\phi_p(-1)p^2 \sum_{j=\frac{p+1}{2}}^{p-2} \frac{\Gamma_p(\frac{1}{2}+j)^2}{\Gamma_p(1+j)^2} (\tfrac{1}{2}+j)^2 \omega^{\frac{3p-3}{2}-j}(\lambda).$$

By repeated use of Proposition 2.4 (2) we have for $\frac{p+1}{2} \leq j \leq p-2$ that

$$\Gamma_p\Big(\frac{1}{2}+\frac{p+1}{2}\Big)^2 \equiv 1 \pmod p$$
$$\Gamma_p\Big(\frac{1}{2}+\frac{p+1}{2}+1\Big)^2 \equiv \Big(\frac{p+2}{2}\Big)^2 \pmod p$$
$$\Gamma_p\Big(\frac{1}{2}+\frac{p+1}{2}+2\Big)^2 \equiv \Big(\frac{p+4}{2}\Big)^2\Big(\frac{p+2}{2}\Big)^2 \pmod p$$
$$\vdots$$
$$\Gamma_p\Big(\frac{1}{2}+p-2\Big)^2 \equiv \Big(\frac{2p-5}{2}\Big)^2\Big(\frac{2p-7}{2}\Big)^2\cdots\Big(\frac{p+2}{2}\Big)^2 \pmod p.$$

By Proposition 2.4 (3), $\Gamma_p(1+j)^2=(j!)^2$. Also using the fact that $\lambda^{p-1}\equiv 1 \pmod p$, we have

$$\begin{aligned}\omega^{\frac{3p-3}{2}-j}(\lambda) &\equiv \lambda^{\frac{3p-3}{2}-j} \pmod p\\ &\equiv \lambda^{\frac{p-1}{2}+p-1-j} \pmod p\\ &\equiv \lambda^{\frac{p-1}{2}-j} \pmod p\end{aligned}$$

for $\frac{p+1}{2}\le j\le p-2$ and thus

$$\begin{aligned}&\sum_{j=\frac{p+1}{2}}^{p-2}\frac{\Gamma_p(\frac{1}{2}+j)^2}{\Gamma_p(1+j)^2}(\tfrac{1}{2}+j)^2\omega^{\frac{3p-3}{2}-j}(\lambda)\\ &\equiv \frac{1}{(\frac{p+1}{2})!^2}\Big(\frac{p}{2}+1\Big)^2\omega^{p-2}(\lambda)\\ &+\ldots+\frac{(\frac{p+2}{2})^2\cdots(\frac{2p-5}{2})^2}{(p-2)!^2}\Big(\frac{1}{2}+p-2\Big)^2\omega^{\frac{p+1}{2}}(\lambda) \pmod p\\ \\ &\equiv \frac{1}{-\phi_p(-1)(\frac{1}{2})}(1)^2\lambda^{-1}\\ &+\cdots+\frac{(1)^2(2)^2\cdots(\frac{p-5}{2})^2}{-\phi_p(-1)(p-2)^2(p-3)^2\cdots(\frac{p+1}{2})^2}\Big(\frac{p-3}{2}\Big)^2\lambda^{-1-\frac{p-5}{2}} \pmod p\\ &\equiv -\phi_p(-1)D(p,\lambda) \pmod p.\end{aligned}$$

This proves the result for $n=1$. □

Remark 3.3. In general it would be beneficial to determine ${}_{n+1}F_n(\lambda) \pmod{p^m}$ for $m\ge 4$.

4. Proofs of Theorems 1.2, 1.4, and 1.6

Proof of Theorem 1.2. Ahlgren and Ono proved (see Theorem 6 in [2]) that

$$a(p) = -p^3{}_4F_3(1) - p.$$

Upon taking $n = 3$ in Theorem 3.2, we have

$$a(p) \equiv p^2 X(p,1,3) + p\Big(Y(p,1,3) - 1\Big) + Z(p,1,3) \pmod{p^3}$$

where

$$X(p,1,3) = \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}^2 \binom{\frac{p-1}{2}}{j}^2 \Bigg(1 + 8j\Big(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j\Big)$$
$$+ j^2\Big(8\Big(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j\Big)^2 - 2\Big(H^{(2)}_{\frac{p-1}{2}+j} - H^{(2)}_j\Big)\Big)\Bigg),$$

$$Y(p,1,3) = \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}^2 \binom{\frac{p-1}{2}}{j}^2 \Bigg(1+4j\Big(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_j\Big)$$
$$- 2j\Big(H^{(1)}_{\frac{p-1}{2}+j} - H^{(1)}_{\frac{p-1}{2}-j}\Big)\Bigg),$$

and

$$Z(p,1,3) = \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^4 16^{-2j}.$$

By the proof of Lemma 7.2 in [2], we know that

$$A\Big(\frac{p-1}{2}\Big) = \sum_{j=0}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j+\frac{p}{2})^2\ \Gamma_p(\frac{1}{2}+j-\frac{p}{2})^2}{\Gamma_p(1+j)^4}.$$

Notice that Proposition 2.5 (2) yields

$$\Gamma_p(\tfrac{1}{2}+j+\tfrac{p}{2})\Gamma_p(\tfrac{1}{2}+j-\tfrac{p}{2}) \equiv \Big\{\Gamma_p(\tfrac{1}{2}+j+\tfrac{p}{2}) + \tfrac{p}{2}\Gamma_p'(\tfrac{1}{2}+j)$$
$$+ \tfrac{p^2}{8}\Gamma_p''(\tfrac{1}{2}+j)\Big\}\Big\{\Gamma_p(\tfrac{1}{2}+j+\tfrac{p}{2}) - \tfrac{p}{2}\Gamma_p'(\tfrac{1}{2}+j) + \tfrac{p^2}{8}\Gamma_p''(\tfrac{1}{2}+j)\Big\} \pmod{p^3}$$

and thus

(20)
$$A\Big(\frac{p-1}{2}\Big) \equiv \sum_{j=0}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^4}{\Gamma_p(1+j)^4} + \frac{p^2}{2}\frac{\Gamma_p(\frac{1}{2}+j)^4}{\Gamma_p(1+j)^4}\Big(G_2(\tfrac{1}{2}+j) - G_1(\tfrac{1}{2}+j)\Big) \pmod{p^3}.$$

By Proposition 3.1 in [13],

$$X(p,1,3) \equiv 0 \pmod{p},$$

$$Y(p,1,3) - 1 \equiv 0 \pmod{p^2}$$

and

$$Z(p,1,3) \equiv \sum_{j=0}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^4}{\Gamma_p(1+j)^4} \pmod{p^3}.$$

Thus by (20)

$$a(p) \equiv A\Big(\frac{p-1}{2}\Big) + \frac{p^2}{2}\sum_{j=0}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^4}{\Gamma_p(1+j)^4}\Big(G_1(\tfrac{1}{2}+j) - G_2(\tfrac{1}{2}+j)\Big) \pmod{p^3}.$$

Finally, an application of Proposition 2.4 yields

$$\frac{\Gamma_p(\frac{1}{2}+j)^4}{\Gamma_p(1+j)^4} \equiv \binom{\frac{p-1}{2}+j}{j}^2 \binom{\frac{p-1}{2}}{j}^2 \pmod{p}$$

and the result is proven. □

Proof of Theorem 1.4. The cases $p=3$ and $p=5$ can be verified directly and so we assume that $p \geq 7$. By Proposition 2.3, we have

$$\left(\frac{-4}{p}\right) = -p \cdot {}_2F_1(1)$$

and so by Theorem 3.2, it is enough to show that

(21) $$X(p,1,1) \equiv C(p) \pmod{p},$$

(22) $$Y(p,1,1) \equiv E(p) \pmod{p^2},$$

$$Z(p,1,1) \equiv \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^2 16^{-j} \pmod{p^3}, \tag{23}$$

$$D(p,1) \equiv D(p) \pmod{p}. \tag{24}$$

We first study $X(p,1,1)$. We have

$$X(p,1,1) = \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}(-1)^j\Big(1+4j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)+ \\ j^2\Big(2\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)^2-\Big(H^{(2)}_{\frac{p-1}{2}+j}-H^{(2)}_j\Big)\Big)\Big).$$

For positive integers n, the identity

(25)

$$\sum_{j=1}^{n}(-1)^j\binom{n+j}{j}\binom{n}{j}\Big(1+4j\big(H^{(1)}_{n+j}-H^{(1)}_j\big)+j^2\big(H^{(1)}_{n+j}-H^{(1)}_j\big)^2-j^2\big(H^{(2)}_{n+j}-H^{(2)}_j\big)\Big) \\ = (1+n)^2(-2-2n+n^2)\frac{(n!)^2(-1)^n}{2(2+2n)!}+\frac{1}{4}(n+1)(4+8n+3n^2+3n^3)(-1)^n- \\ \frac{1}{2}(-1+n+n^2)+\frac{3}{2}n^2(1+n)^2(-1)^n\sum_{i=1}^{n}\frac{i!^2}{(2+2i)!}+n^2(1+n)^2(-1)^n\sum_{i=1}^{n}\frac{(-1)^i}{i^2}.$$

was discovered using Sigma (see Section 5). Taking $n=\frac{p-1}{2}$ in (25) and reducing mod p, one can check that $X(p,1,1)\equiv C(p) \pmod{p}$. This proves (21).

We now consider $Y(p,1,1)$. By definition, we have

$$Y(p,1,1) = \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}(-1)^j\Bigg(1+j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big) \\ +j\Big(H^{(1)}_{\frac{p-1}{2}-j}-H^{(1)}_j\Big)\Bigg).$$

For positive integers n, the relation

$$\begin{aligned}\sum_{j=1}^{n}\binom{n+j}{j}\binom{n}{j}(-1)^j\left(1+j\left(H_{n+j}^{(1)}+H_{n-j}^{(1)}-2H_j^{(1)}\right)\right)\\ =(1+2n)\binom{2n}{n}(-1)^n-\frac{3}{2}n(1+n)(-1)^n\sum_{i=1}^{n}\frac{\binom{2i}{i}}{i}\end{aligned} \tag{26}$$

was discovered again using Sigma (see Section 5). Taking $n=\frac{p-1}{2}$ in (26) and reducing mod p^2, we have that $Y(p,1,1)\equiv E(p) \pmod{p^2}$. This proves (22). Finally, by (19) and the definition of $D(p,\lambda)$, then (23) and (24) and thus Theorem 1.2 follows. $\square$

Remark 4.1. As we mentioned in the introduction, one can not directly use the clever methods from Section 4 in [13] to compute $X(p,1,1)$ mod p. Let us be more specific. For $l\in\mathbb{Z}$ and $n\in\mathbb{N}$ we define

$$(l)_n := \begin{cases} 1 & \text{if } n=0,\\ l(l+1)(l+2)\cdots(l+n-1) & \text{if } n\geq 1.\end{cases}$$

Also, let us define

$$Q(z):=\frac{z}{2}\frac{d^2}{dz^2}\left[z(z+1)^2_{\frac{p-1}{2}}\right]=\sum_{k=0}^{p-1}a_k z^k$$

with $a_k\in\mathbb{Z}$. A short computation yields

$$(j+1)^2_{\frac{p-1}{2}}\equiv\frac{\Gamma_p(\frac{1}{2}+j)^2}{\Gamma_p(1+j)^2}\pmod{p}$$

and

$$\begin{aligned}Q(j)\equiv(j+1)^2_{\frac{p-1}{2}}\Bigg(2j^2\left(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\right)^2\\ -j^2\left(H^{(2)}_{\frac{p-1}{2}+j}-H^{(2)}_j\right)+2j\left(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\right)\Bigg) \bmod p\end{aligned}$$

and thus, via Lemma 2.6, an evaluation of $X(p,1,1)$ mod p follows from that of $\sum_{j=1}^{\frac{p-1}{2}}Q(j)$ mod p. We then have

$$\begin{aligned}\sum_{j=1}^{p-1} Q(j) &= \sum_{j=1}^{p-1}\sum_{k=1}^{p-1} a_k j^k\\ &= \sum_{k=1}^{p-1} a_k \sum_{j=1}^{p-1} j^k\\ &\equiv -a_{p-1} \pmod p.\end{aligned}$$

Here we have used the fact that $j \mid Q(j)$ and thus $a_0 = 0$ and the standard exponential sum evaluation

$$\sum_{j=1}^{p-1} j^k = \begin{cases} -1 \pmod p & \text{if } (p-1) \mid k,\\ \;\;\,0 \pmod p & \text{otherwise.}\end{cases}$$

If we write

$$Q(z) = \frac{z}{2}\frac{d^2}{dz^2}\Big[z^p + \cdots\Big] = \frac{z}{2}\big(p(p-1)z^{p-2} + \cdots\big),$$

then we deduce that $\sum_{j=1}^{p-1} Q(j) \equiv 0 \pmod p$. From this result, we can not deduce an explicit evaluation of $\sum_{j=1}^{\frac{p-1}{2}} Q(j)$ due to the fact that $Q(j) \not\equiv 0 \pmod p$ for $\frac{p-1}{2} < j < p$. It is for this reason that we resort to the present calculations.

Proof of Theorem 1.6. Loh and Rhodes have shown (see also [15] or Theorem 1 in [22]) that

$$_2a_1(p;\lambda) = -\phi_p(-\lambda)p_2F_1(\lambda^{-1}). \tag{27}$$

The result then follows by taking λ^{-1} and $n = 1$ in Theorem 3.2 and applying (27). □

5. Finding and proving identities (25) and (26)

Using the algorithms presented in [33, 26] hypergeometric sum identities such as

$$\sum_{k=0}^{n} (-1)^k \binom{n+k}{k}\binom{n}{k} = (-1)^n \tag{28}$$

can be discovered and proven with the computer. More generally, with the summation package Sigma [30] one can attack multi-sum identities involving indefinite nested sum and product expressions. In particular, our sum identities (25) and (26) fit perfectly in the input class of Sigma. For simplicity, we write H_k for $H_k^{(1)}$ throughout this section.

5.1. **Identity** (26)**.** Using our algorithms we can derive the following harmonic sum identities:

(29)
$$\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}\binom{n}{k}H_k=\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}\binom{n}{k}H_{n+k}=(-1)^n2H_n,$$

(30)
$$\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}\binom{n}{k}kH_k=(-1)^n n(n+1)(2H_n-1),$$

(31)
$$\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}\binom{n}{k}kH_{n+k}=(-1)^n n(n+1)2H_n-(-1)^n n^2,$$

and

(32)
$$\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}\binom{n}{k}kH_{n-k}=-(-1)^n(n+1)^2+(-1)^n(2n+1)\binom{2n}{n}$$
$$+2n(n+1)(-1)^nH_n-\frac{3}{2}n(n+1)(-1)^n\sum_{i=1}^{n}\frac{\binom{2i}{i}}{i}.$$

Then, combining (28), (31) and (32) we arrive at identity (26). We can find and prove the identities (28)–(32) always by the same mechanism: Compute a recurrence by the creative telescoping paradigm, solve the recurrence, and combine the solutions to get a closed form for the input sum. Subsequently, we illustrate these steps with identity (32). After loading the package

In[1]:= $<<$ **Sigma.m**
Sigma - A summation package by Carsten Schneider © RISC-Linz

into the computer algebra system Mathematica, we insert the sum in question:

In[2]:= $\mathbf{S = SigmaSum[SigmaPower[-1, k]kSigmaBinomial[n+k, k]}$
$\mathbf{SigmaBinomial[n, k]SigmaHNumber[n-k], \{k, 0, n\}]}$

Out[2]= $\sum_{k=0}^{n}(-1)^k k\binom{n+k}{k}\binom{n}{k}H_{n-k}$

Remark 5.1. Various functions support the user, like `SigmaSum` for sums, `SigmaPower` for powers, `SigmaBinomial` for binomials, or `SigmaHNumber` for harmonic numbers.

Next, we compute a recurrence relation for the given sum `S` by inputting:

In[3]:= **rec = GenerateRecurrence**[S]

Out[3]= $(n+2)(2n+1)(n+1)^2\mathrm{SUM}[n+2]+2(n+3)(2n^2+4n+1)(n+1)\mathrm{SUM}[n+1]+$
$(n+1)(n+2)(n+3)(2n+3)\mathrm{SUM}[n] == -(2n+1)(2n+3)(3n+1)(3n+4)(-1)^n\binom{2n}{n}$

This means that SUM[n](= $\mathtt{S}=\sum_{k=0}^{n}(-1)^k k\binom{n+k}{k}\binom{n}{k}H_{n-k}$) satisfies Out[3].

Proof of Out[3]: Define $f(n,k) := (-1)^k k\binom{n+k}{k}\binom{n}{k}H_{n-k}$. The correctness follows by the creative telescoping equation

(33) $g(n,k+1)-g(n,k)=c_0(n)f(n,k)+c_1(n)f(n+1,k)+c_2(n)f(n+2,k)$

and the proof certificate $c_0(n)=(n+2)(n+3)(2n+3)$, $c_1(n)=2(n+3)\left(2n^2+4n+1\right)$, $c_2(n)=(n+1)(n+2)(2n+1)$ and

$$g(n,k)=(k-1)k^2(2H_{n-k}(k-n-2)(k-n-1)(n+1)(k(4n+7)-2(2n^3+10n^2+17n+10))+$$
$$(-k-n-1)(16n^4+88n^3+179n^2+163n+2k^2(4n^2+11n+7)-k(24n^3+$$
$$98n^2+131n+59)+58))(-1)^k\binom{n+k}{k}\binom{n}{k}\Big/\left((n+1)(-k+n+1)^2(-k+n+2)^2\right).$$

We verify (33) as follows. Express $g(n,k+1)$ in terms of $h(n,k)=(-1)^k\binom{n+k}{k}\binom{n}{k}$ and H_{n-k} by using the relations

$$h(n,k+1)=-\frac{(n-k)(n+k+1)}{(k+1)^2}h(n,k)$$

and

$$H_{n-k-1}=H_{n-k}-\frac{1}{n-k}.$$

Similarly, express $f(n+i,k)$ in terms of $h(n,k)$ and H_{n-k} by using the relations

$$h(n+1,k)=\frac{n+k+1}{n-k+1}h(n,k)$$

and

$$H_{n-k+1} = H_{n-k} + \frac{1}{n-k+1}.$$

Then (33) can be checked directly. Summing (33) over k from 0 to n produces Out[3]. □

Next, we solve the recurrence relation Out[3] by typing in:

In[4]:= **recSol = SolveRecurrence[rec[[1]], SUM[n]]**

Out[4]= $\{\{0, \mathtt{n}(1+\mathtt{n})(-1)^{\mathtt{n}}\}, \{0, (1+\mathtt{n})(-1)^{\mathtt{n}}\big(-1+2\mathtt{n}\sum_{\mathtt{i}=1}^{\mathtt{n}}\frac{1}{\mathtt{i}}\big)\},$
$\{1, -\frac{1}{2}(-1)^{\mathtt{n}}\big(-2(1+2\mathtt{n})\binom{2\mathtt{n}}{\mathtt{n}} + 3\mathtt{n}(1+\mathtt{n})\sum_{\mathtt{i}=1}^{\mathtt{n}}\frac{\binom{2\mathtt{i}}{\mathtt{i}}}{\mathtt{i}}\big)\}\}$

The result has to be interpreted as follows. Sigma finds two linearly independent solutions $h_1(n) = n(1+n)(-1)^n$ and $h_2(n) = (1+n)(-1)^n\big(-1+2n\sum_{i=1}^{n}\frac{1}{i}\big)$ of the the homogeneous version of Out[3] (indicated by the 0 in front) plus one particular solution

$$p(n) = -\frac{1}{2}(-1)^n\big(-2(1+2n)\binom{2n}{n} + 3n(1+n)\sum_{i=1}^{n}\frac{\binom{2i}{i}}{i}\big)$$

of the input recurrence itself (indicated by the 1 in front). The correctness of the result can be easily verified by using, e.g., the relation

$$\sum_{i=1}^{n+1}\binom{2i}{i}\frac{1}{i} = \sum_{i=1}^{n}\binom{2i}{i}\frac{1}{i} + \frac{2(2n+1)}{(n+1)^2}\binom{2n}{n}.$$

Finally, by taking all linear combinations $c_1h_1(n) + c_2h_2(n) + p(n)$ for constants c_1 and c_2, free of n, we obtain all solutions of Out[3]. Hence, by considering the first two initial values of S we can discover and prove (32):

In[5]:= **FindLinearCombination[recSol, S, 2]**

Out[5]= $-(-1)^{\mathtt{n}}(1+\mathtt{n})^2+(-1)^{\mathtt{n}}(1+2\mathtt{n})\binom{2\mathtt{n}}{\mathtt{n}}+2\mathtt{n}(1+\mathtt{n})(-1)^{\mathtt{n}}\sum_{\mathtt{i}=1}^{\mathtt{n}}\frac{1}{\mathtt{i}}-\frac{3}{2}\mathtt{n}(1+\mathtt{n})(-1)^{\mathtt{n}}\sum_{\mathtt{i}=1}^{\mathtt{n}}\frac{\binom{2\mathtt{i}}{\mathtt{i}}}{\mathtt{i}}$

Remark 5.2. Looking at the identities (28)–(32) one immediately sees that the combination (28) + 2 · (31) − 2 · (30) produces the identity

$$\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}\binom{n}{k}\Big(1+2k\Big(H_{n+k}-H_k\Big)\Big) = (-1)^n(2n+1)$$

which has been proven by Sigma in [18, Lemma 2.2]. In particular, we find [18, Proposition 2.6]

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j}\binom{\frac{p-1}{2}}{j}(-1)^j\Big(1+2j\Big(H^{(1)}_{\frac{p-1}{2}+j}-H^{(1)}_j\Big)\Big) \equiv 0 \pmod{p}.$$

Since the sums can be combined so nicely, we had also the hope to find a solution for the sum

$$S_\lambda(n) := \sum_{k=0}^{n}(-\lambda)^k\binom{n+k}{k}\binom{n}{k}\Big(1+2k\Big(H_{n+k}-H_k\Big)\Big)$$

which is related to the Theorems 1.5 and 1.6. Sigma was able to compute the recurrence

$$\begin{aligned}(n+2)^2 S_\lambda(n) &+ (2\lambda-1)\left(4n^2+18n+21\right)S_\lambda(n+1)\\ &+\left(16n^2\lambda^2+80n\lambda^2+100\lambda^2-16n^2\lambda-80n\lambda-100\lambda+6n^2+30n+39\right)S_\lambda(n+2)\\ &+(2\lambda-1)\left(4n^2+22n+31\right)S_\lambda(n+3)+(n+3)^2 S_\lambda(n+4)=0,\end{aligned}$$

but failed to find any solution for a generic value λ. Interesting enough, choosing $\lambda=\frac{1}{2}$ the recurrences gets much simpler. In particular, this indicates that considering the sums $S_{\frac{1}{2}}(2n)$ and $S_{\frac{1}{2}}(2n+1)$ separately, one can compute recurrences of order 2 for each of them. Indeed, applying the mechanism from above for each of the sums gives (two different) recurrences of order two. Luckily, we can even solve the recurrences which yields

$$S_{\frac{1}{2}}(2n) = \frac{(-1)^n 2^{2n}(n!)^2}{(2n)!}$$

and

$$S_{\frac{1}{2}}(2n+1) = \frac{(-1)^n(2n)!}{2^{2n}(n!)^2}\Big((2n+1)\big(H_n-H_{2n}\big)-1\Big).$$

The sums $S_\lambda(n)$ occur in a certain combinatorial expression for $\binom{p-1}{(p-1)/2}^2$ modulo p^2 which appears in [24]. For more details on how the explicit evaluation of this expression is related to the infinitude of non-Wieferich primes, please see [24].

5.2. **Identity** (25). Finally, we consider the sum

In[6]:= $$\mathbf{mySum} = \sum_{\mathbf{k=0}}^{\mathbf{n}}(-1)^{\mathbf{k}}\binom{\mathbf{n+k}}{\mathbf{k}}\binom{\mathbf{n}}{\mathbf{k}}\Big(\mathbf{2k^2}\Big(\mathbf{H_{n+k}}-\mathbf{H_k}\Big)^{\mathbf{2}}-\mathbf{k^2}\Big(\mathbf{H^{(2)}_{n+k}}-\mathbf{H^{(2)}_k}\Big)\Big)$$

One option is to follow the same strategy as above: We can compute a recurrence of order 4 for `mySum` and can solve the derived recurrence to find the right hand side of (35). But, since this recurrence relation is rather big, and the proof certificate is even bigger (it fills about one page), we follow a refined strategy presented in [25] and [31]. Namely, by running our creative telescoping algorithm with the additional option `SimplifyByExt` $\rightarrow$ `DepthNumber` we can find a recurrence of smaller order (order one!):

In[7]:= **rec = GenerateRecurrence[mySum, SimplifyByExt → DepthNumber]**

Out[7]= $2(2n+1)(n+2)^2\mathtt{SUM}[n]2(2n+1)n^2\mathtt{SUM}[n+1] ==$

$$4(1+4n)+n^2(n+1)(n+2)(3n+2)\sum_{i=0}^{n}\frac{(-1)^i\binom{n+i}{i}\binom{n}{i}}{(n+i)^2}+$$
$$2n\left(4n^2+3n-4\right)(2n+1)\sum_{i=0}^{n}(-1)^i\binom{n+i}{i}\binom{n}{i}+$$
$$8(n-1)n(n+1)(n+2)(2n+1)\Big(\sum_{i=0}^{n}(-1)^i\binom{n+i}{i}\binom{n}{i}H_{n+i}-\sum_{i=0}^{n}(-1)^i\binom{n+i}{i}\binom{n}{i}H_i\Big)$$

Proof of Out[7]: Define $f(n,k)=(-1)^k\binom{n+k}{k}\binom{n}{k}\big(2k^2\big(H_{n+k}-H_k\big)^2-k^2\big(H^{(2)}_{n+k}-H^{(2)}_k\big)\big)$. Then the correctness of Out[7] follows by the creative telescoping equation

$$g(n,k+1)-g(n,k)=c_0(n)f(n,k)+c_1(n)f(n+1,k) \tag{34}$$

with the proof certificate $c_0(n)=2(n+2)^2(2n+1)$, $c_1(n)=2n^2(2n+1)$ and

$$g(n,k)=\Bigg(4(k-1)^2n(n+1)^2(2n+1)k^2\Big(2H_k^2-4H_{n+k}H_k+2H_{n+k}^2+H_k^{(2)}-H_{n+k}^{(2)}\Big)-$$
$$\Big(n(n+2)k^3-(n^3+2n^2+2n+2)k^2-(n+1)^2(n^2-2)k+n(n+1)^2(n^2+n-2)\Big)8n(n+1)$$
$$(2n+1)\Big(H_k-H_{n+k}\Big)+(16n^5+48n^4+29n^3+14n^2+20n+8)k^2+n(n+1)^2(16n^4+23n^3+$$
$$n^2+12n+8)-(32n^6+101n^5+98n^4+55n^3+54n^2+36n+8)k\Bigg)\frac{(-1)^k\binom{n+k}{k}\binom{n}{k}}{(1-k+n)n(1+n)}+$$
$$n^2(n+1)(n+2)(3n+2)\sum_{i=0}^{k}\frac{(-1)^i\binom{n+i}{i}\binom{n}{i}}{(n+i)^2}+2n\left(4n^2+3n-4\right)(2n+1)\sum_{i=0}^{k}(-1)^i\binom{n+i}{i}\binom{n}{i}$$
$$+8(n-1)n(n+1)(n+2)(2n+1)\Big(\sum_{i=0}^{k}(-1)^i\binom{n+i}{i}\binom{n}{i}H_{n+i}-\sum_{i=0}^{k}(-1)^i\binom{n+i}{i}\binom{n}{i}H_i\Big)$$

Since the sums and products inside of $g(n,k)$ are all indefinite, e.g., we can apply the relation

$$\sum_{i=0}^{k+1}(-1)^i\binom{n+i}{i}\binom{n}{i}=\sum_{i=0}^{k}(-1)^i\binom{n+i}{i}\binom{n}{i}-(-1)^k\tfrac{(k-n)(k+n+1)}{(k+1)^2}\binom{n+k}{k}\binom{n}{k},$$

the verification of (34) is immediate. Summing (34) over k from 0 to n produces Out[7]. $\square$

At first glance the recurrence Out[7] seems to be disappointing: we start with the definite sum `mySum`, and end up with a recurrence again involving definite sums. But, these sums are much simpler than the input sum. In particular, we already derived closed forms in (28) and (29). Together with

$$\sum_{i=0}^{n}(-1)^i\frac{\binom{n+i}{i}\binom{n}{i}}{(n+i)^2}=-(-1)^n\frac{n!^2}{n^2(2n)!},$$

which we also find easily with Sigma, we end up at

In[8]:= $\mathbf{rec = rec/.\{\sum_{i=0}^{n}(-1)^i\frac{\binom{n+i}{i}\binom{n}{i}}{(n+i)^2}\to -(-1)^n\frac{n!^2}{n^2(2n)!},}$
$\mathbf{\sum_{i=0}^{n}(-1)^i\binom{n+i}{i}\binom{n}{i}H_i\to\sum_{i=0}^{n}(-1)^i\binom{n+i}{i}\binom{n}{i}H_{n+i}\}}$

Out[8]= $2(2n+1)n^2\mathrm{SUM}[n+1]+2(n+2)^2(2n+1)\mathrm{SUM}[n]==$
$4(2n+1)-\frac{(-1)^n(n+1)(n+2)(3n+2)(n!)^2}{(2n)!}+2(-1)^n n(2n+1)\left(4n^2+3n-4\right).$

Given this recurrence, one can directly read off its solution. With some simplifications Sigma yields:

In[9]:= **recSol = SolveRecurrence[rec[[1]], SUM[n], SimpleSumRepresentation → True]**

Out[9]= $\{\{0,(-1)^n n^2(n+1)^2,\{1,(1+n)^2(-2-2n+n^2)\frac{(n!)^2(-1)^n}{2(2+2n)!}-\frac{1}{2}(-1+n+n^2)+$
$\frac{1}{4}n(-4+11n+6n^2+3n^3)(-1)^n+\frac{3}{2}n^2(1+n)^2(-1)^n\sum_{i=1}^{n}\frac{i!^2}{(2+2i)!}+n^2(1+n)^2(-1)^n\sum_{i=1}^{n}\frac{(-1)^i}{i^2}\}\}$

Looking at the first initial values we end up at the identity

(35)
$$\begin{aligned}\sum_{k=1}^{n}\binom{n+k}{k}\binom{n}{k}(-1)^k&\left(2k^2\left(H_{n+k}-H_k\right)^2-k^2\left(H^{(2)}_{n+k}-H^{(2)}_k\right)\right)\\ =&(1+n)^2(-2-2n+n^2)\frac{(n!)^2(-1)^n}{2(2+2n)!}+\tfrac{1}{4}n(-4+11n+6n^2+3n^3)(-1)^n\\ &-\tfrac{1}{2}(-1+n+n^2)+\tfrac{3}{2}n^2(1+n)^2(-1)^n\sum_{i=1}^{n}\tfrac{i!^2}{(2+2i)!}+n^2(1+n)^2(-1)^n\sum_{i=1}^{n}\tfrac{(-1)^i}{i^2}.\end{aligned}$$

To this end, using in addition (28), (30) and (31) we obtain identity (25).

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