

GAUSSIAN HYPERGEOMETRIC SERIES AND SUPERCONGRUENCES

ROBERT OSBURN AND CARSTEN SCHNEIDER

ABSTRACT. Let p be an odd prime. In 1984, Greene introduced the notion of hypergeometric functions over finite fields. Special values of these functions have been of interest as they are related to the number of \mathbb{F}_p points on algebraic varieties and to Fourier coefficients of modular forms. In this paper, we explicitly determine these functions modulo higher powers of p and discuss an application to supercongruences. This application uses two non-trivial generalized Harmonic sum identities discovered using the computer summation package *Sigma*. We illustrate the usage of *Sigma* in the discovery and proof of these two identities.

1. INTRODUCTION

In [16] and [17], Greene defined general hypergeometric series over finite fields. His aim was to show that these functions satisfy properties analogous to classical hypergeometric series. For example, the four major evaluations of the ordinary hypergeometric series ${}_3F_2$ due to Saalschütz, Dixon, Watson, and Whipple [5] all have finite field interpretations (see page 126 of [16]). Greene's work was in part motivated by the analogy between Gauss sums and Gamma functions [10], [23], [43].

His approach has proven to be a powerful technique for character sum evaluations. Recently, several authors have shown that special values of these functions are related to the number of points over \mathbb{F}_p , p an odd prime, of Calabi-Yau threefolds [3], traces of Hecke operators [11], formulas for Ramanujan's τ -function [35], and the number of points on a family of elliptic curves [13]. We should also mention that hypergeometric series over arbitrary fields has been developed [14], [15], but their application to number theory has yet to be investigated.

The purpose of this paper is to further study arithmetic properties of hypergeometric functions over finite fields. In particular, we explicitly determine these functions modulo higher powers of p and then briefly discuss extensions of supercongruences.

We first recall some definitions. 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 [16] and [17], we give two definitions. The first definition is the finite field analogue of the binomial coefficient. If A and B are characters of \mathbb{F}_p , then

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

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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. If A_0, A_1, \dots, A_n , and B_1, \dots, B_n are characters of \mathbb{F}_p , then the Gaussian hypergeometric function over \mathbb{F}_p is defined by

$$(2) \quad {}_{n+1}F_n \left(\begin{matrix} A_0, & A_1, & \dots, & A_n \\ & B_1, & \dots, & B_n \end{matrix} \middle| x \right)_p := \frac{p}{p-1} \sum_{\chi} \binom{A_0\chi}{\chi} \binom{A_1\chi}{B_1\chi} \cdots \binom{A_n\chi}{B_n\chi} \chi(x),$$

where the summation is over all characters χ of \mathbb{F}_p . In this paper, 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 ${}_{n+1}F_n(\lambda)$. By [16] and [17], $p^n {}_{n+1}F_n(\lambda) \in \mathbb{Z}$. Before stating the main result, we recall that for $i, n \in \mathbb{N}$, generalized Harmonic sums $H_n^{(i)}$ are defined by

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

and $H_0^{(i)} := 0$. We now define the quantities

$$(3) \quad X(p, \lambda, n) := \phi_p(\lambda) \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2} + j}{j}^l \binom{\frac{p-1}{2}}{j}^l (-1)^{jl} \lambda^{-j} \left(1 + 2(n+1)j \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right) \right. \\ \left. + j^2 \left(\frac{n+1}{2} (1+n) \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right)^2 - \left(\frac{n+1}{2} \right) \left(H_{\frac{p-1}{2}+j}^{(2)} - H_j^{(2)} \right) \right) \right),$$

$$(4) \quad Y(p, \lambda, n) := \phi_p(\lambda) \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2} + j}{j}^l \binom{\frac{p-1}{2}}{j}^l (-1)^{jl} \lambda^{-jp} \left(1 + (n+1)j \left(H_{\frac{p-1}{2}+j}^{(1)} \right. \right. \\ \left. \left. - H_j^{(1)} \right) - \left(\frac{n+1}{2} \right) j \left(H_{\frac{p-1}{2}+j}^{(1)} - H_{\frac{p-1}{2}-j}^{(1)} \right) \right),$$

$$(5) \quad Z(p, \lambda, n) := \phi_p(\lambda) \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^{2l} 16^{-jl} \lambda^{-jp^2},$$

and

$$(6) \quad D(p, \lambda) := \sum_{j=0}^{\frac{p-5}{2}} \frac{j!^2}{\prod_{i=0}^j (i + \frac{1}{2})^2} (j+1)^2 \lambda^{-j-1},$$

where $l := \frac{n+1}{2}$. The main result of this paper is the following.

Theorem 1.1. *If $n \geq 2$, then*

$$(7) \quad -p^n {}_{n+1}F_n(\lambda) \equiv (-\phi_p(-1))^{n+1} \left[p^2 X(p, \lambda, n) + pY(p, \lambda, n) + Z(p, \lambda, n) \right] \pmod{p^3}$$

and if $n = 1$, then

$$(8) \quad -p {}_2F_1(\lambda) \equiv p^2 \left[X(p, \lambda, 1) + D(p, \lambda) \right] + pY(p, \lambda, 1) + Z(p, \lambda, 1) \pmod{p^3}.$$

We note that Theorem 1.1 generalizes both Theorem 1 in [1], where the case $n = 2$ was handled modulo p^2 , and Theorem 2.4 in [25]. As an application of Theorem 1.1, we prove a supercongruence for the Legendre symbol $\left(\frac{-1}{p}\right)$. This result generalizes Theorem 1 in [27].

Corollary 1.2. *Let p be an odd prime. Then*

$$(9) \quad \sum_{n=0}^{\frac{p-1}{2}} \binom{2n}{n}^2 16^{-n} + \frac{3}{8} p(-1)^{\frac{p-1}{2}} \sum_{i=1}^{\frac{p-1}{2}} \binom{2i}{i} \frac{1}{i} \equiv \left(\frac{-1}{p}\right) \pmod{p^3}.$$

The method of proof for Theorem 1.1 has its origin in [3]. Namely, the idea is to first observe that since the functions ${}_{n+1}F_n(\lambda)$ are defined in terms of Jacobi sums, then one can express them as Gauss sums. One then applies the Gross-Koblitz formula [18] to express the Gauss sums in terms of p -adic Gamma functions. Using combinatorial properties of the p -adic Gamma function, Theorem 1.1 then follows. For an introduction to these methods, see [32]. This general framework has been the basis for several recent results on supercongruences (see [1], [21], [25], [27], [28], [29]). Theorem 1.1 has recently been used to settle a conjecture of van Hamme (see [26]). Finally, the congruence in (9) appears to hold modulo p^4 . This has been numerically confirmed for all primes less than 5000.

The paper is organized as follows. In Section 2, we recall properties of the p -adic Gamma function. In Section 3, we prove Theorem 1.1. In Section 4, we prove Corollary 1.2 using Theorem 1.1 and two non-trivial Harmonic sum identities discovered using the computer summation program Sigma [39]. 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 [33]. These types of identities played an important role in the proof of Beukers' supercongruence for Apéry numbers (see [2] or Theorem 7 in [3]).

2. PRELIMINARIES

We first recall the definition of the p -adic Gamma function and list some of its main properties. For more details, see [22], [30], or [37]. 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

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

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

Proposition 2.1. *Let $n \in \mathbb{N}$ and $x \in \mathbb{Z}_p$. Then*

- (1) $\Gamma_p(0) = 1$.
- (2) $\frac{\Gamma_p(x+1)}{\Gamma_p(x)} = \begin{cases} -x & \text{if } |x| = 1, \\ -1 & \text{if } |x| < 1. \end{cases}$
- (3) *If $0 \leq n \leq p-1$, then $n! = (-1)^{n+1} \Gamma_p(n+1)$.*
- (4) $|\Gamma_p(x)| = 1$.
- (5) *Let $x_0 \in [1, 2, \dots, p]$ 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

$$(10) \quad G_1(x) := \frac{\Gamma'_p(x)}{\Gamma_p(x)}$$

and

$$(11) \quad G_2(x) := \frac{\Gamma''_p(x)}{\Gamma_p(x)}.$$

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 [8] or [21].

Proposition 2.2. *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) $\Gamma'_p(x+z) \equiv \Gamma'_p(x) + z\Gamma''_p(x) \pmod{p^2}$.

We also need the following combinatorial congruence which relates Γ_p to certain binomial coefficients.

Lemma 2.3. *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 2.1 (3) and (5), we have

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

Now, using Proposition 2.2 (2), we have

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

and the result follows. □

Finally, we need to define

$$(12) \quad A(j) := G_1\left(\frac{1}{2}+j\right) - G_1(1+j)$$

and for a positive integer n

$$(13) \quad \begin{aligned} B(n, j) &:= \frac{n+1}{2} \left(G_2\left(\frac{1}{2}+j\right) - G_2(1+j) \right) + \frac{(n+1)n}{2} G_1\left(\frac{1}{2}+j\right)^2 \\ &\quad + \frac{(n+1)(n+2)}{2} G_1(1+j)^2 - (n+1)^2 G_1\left(\frac{1}{2}+j\right) G_1(1+j). \end{aligned}$$

We require the following Lemma which relates $A(j)$ and $B(n, j)$ to generalized Harmonic sums. The proof is similar to Lemma 4.1 in [21] and thus is omitted.

Lemma 2.4. *Let p be an odd prime and $0 \leq j \leq \frac{p-1}{2}$. Then*

$$(14) \quad A(j) \equiv H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} + 2p \sum_{r=0}^{j-1} \frac{1}{(2r+1)^2} \pmod{p^2}$$

and

$$(15) \quad B(n, j) \equiv \frac{(n+1)^2}{2} \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right)^2 - \frac{(n+1)}{2} \left(H_{\frac{p-1}{2}+j}^{(2)} - H_j^{(2)} \right) \pmod{p}.$$

3. PROOF OF THEOREM 1.1

We are now in a position to prove Theorem 1.1.

Proof. Let $n \geq 3$ be odd. From (1) and (2), 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 [18] to get (see also [3] or [25])

$$(16) \quad -p^n {}_{n+1}F_n(\lambda) = \frac{1}{1-p} \left\{ \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \left(\sum_{j=0}^{\frac{p-3}{2}} \frac{\Gamma_p(\frac{j}{p-1})^{n+1}}{\Gamma_p(\frac{1}{2} + \frac{j}{p-1})^{n+1}} \omega^j(\lambda) \right. \right. \\ \left. \left. + p^{n+1} \sum_{j=\frac{p+1}{2}}^{p-2} \frac{\Gamma_p(\frac{j}{p-1})^{n+1}}{\Gamma_p(\frac{j}{p-1} - \frac{1}{2})^{n+1}} \omega^j(\lambda) \right) \right\}.$$

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 $s \geq 1$. As $n \geq 3$ is odd, the second sum in (16) 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 2.1 and reindex the summation to obtain

$$(17) \quad -p^n {}_{n+1}F_n(\lambda) \\ \equiv (1 + p + p^2) \left\{ \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2} + j + jp + jp^2)^{n+1}}{\Gamma_p(1 + j + jp + jp^2)^{n+1}} \omega^{\frac{p-1}{2}-j}(\lambda) \right\} \pmod{p^3}.$$

By Proposition 2.2 (2), we see that

$$\Gamma_p(x_0 + j + jp + jp^2)^{n+1} \equiv \Gamma_p(x_0 + j)^{n+1} \left[1 + (n+1)(jp + jp^2)G_1(x_0 + j) \right. \\ \left. + \frac{n+1}{2}(jp + jp^2)^2 \left(G_2(x_0 + j) + nG_1(x_0 + j)^2 \right) \right] \pmod{p^3}$$

for $x_0 \in \mathbb{Z}_p$. We expand the numerator and denominator of (17) with $x_0 = \frac{1}{2}$ and $x_0 = 1$ respectively. After multiplying the numerator and denominator by

$$1 - (n+1)jpG_1(1+j) - \frac{n+1}{2}j^2p^2 \left(G_2(1+j) - (n+2)G_1(1+j)^2 \right) - (n+1)jp^2G_1(1+j),$$

we get

$$\begin{aligned}
& -p^n {}_{n+1}F_n(\lambda) \\
(18) \quad & \equiv (1+p+p^2) \left\{ \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \left(1 + (n+1)jpA(j) \right. \right. \\
& \left. \left. + (n+1)jp^2A(j) + j^2p^2B(n,j) \right) \omega^{\frac{p-1}{2}-j}(\lambda) \right\} \pmod{p^3}
\end{aligned}$$

where $A(j)$ and $B(n, j)$ are defined by (12) and (13). We now need to consider the sums

$$(19) \quad \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \left(1 + 2(n+1)jA(j) + j^2B(n, j) \right) \omega^{\frac{p-1}{2}-j}(\lambda),$$

$$(20) \quad \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \left(1 + (n+1)jA(j) \right) \omega^{\frac{p-1}{2}-j}(\lambda),$$

and

$$(21) \quad \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \omega^{\frac{p-1}{2}-j}(\lambda)$$

which are the coefficients of p^2 , p , and 1 respectively in (18). Observe that as we want to determine ${}_{n+1}F_n(\lambda) \pmod{p^3}$, it suffices to compute (19) \pmod{p} , (20) $\pmod{p^2}$, and (21) $\pmod{p^3}$. Also note that

$$(22) \quad \omega^{\frac{p-1}{2}-j}(\lambda) = \omega^{\frac{p-1}{2}}(\lambda) \omega^{-j}(\lambda) = \phi_p(\lambda) \omega^{-j}(\lambda)$$

as ω is of order $p-1$. By Lemma 4.4 in [21], we see that

$$(23) \quad \left(\frac{n+1}{2}\right)j \left(H_{\frac{p-1}{2}+j}^{(1)} - H_{\frac{p-1}{2}-j}^{(1)} \right) \equiv -2(n+1)jp \sum_{r=0}^{j-1} \frac{1}{(2r+1)^2} \pmod{p^2}.$$

By Lemma 2.3, we have

$$(24) \quad \left[-\phi_p(-1)(-1)^j \binom{\frac{p-1}{2}+j}{j} \binom{\frac{p-1}{2}}{j} \right]^{\frac{n+1}{2}} \equiv \frac{\Gamma_p(\frac{1}{2}+j)^{n+1}}{\Gamma_p(1+j)^{n+1}} \pmod{p^2}$$

and so after combining Lemma 2.4, (22), (23), (24) and accounting for $j=0$, then (19) is congruent modulo p to (3) and (20) is congruent modulo p^2 to (4). 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

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

By Proposition 2.5 in [27], 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 (22), we have that (21) and (5) are congruent modulo p^3 , namely

$$(25) \quad \begin{aligned} \phi_p(\lambda) + (-\phi_p(-1))^{\frac{n+1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\Gamma_p(\frac{1}{2} + j)^{n+1}}{\Gamma_p(1 + j)^{n+1}} \omega^{\frac{p-1}{2}-j}(\lambda) \\ \equiv \phi_p(\lambda) \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^{n+1} 16^{-j(\frac{n+1}{2})} \lambda^{-jp^2} \pmod{p^3}. \end{aligned}$$

This proves the result for $n \geq 3$ odd. A similar argument applies to the case $n \geq 2$ is even. We now turn to the case $n = 1$. By (16), we need only consider the last sum

$$(26) \quad -\phi_p(-1)p^2 \sum_{j=\frac{p+1}{2}}^{p-2} \frac{\Gamma_p(\frac{j}{p-1})^2}{\Gamma_p(\frac{j}{p-1} - \frac{1}{2})^2} \omega^j(\lambda).$$

By (5) and (6) of Proposition 2.1 and after reindexing the exponent of $\omega(\lambda)$, (26) is equivalent modulo p^3 to

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

By repeated use of Proposition 2.1 (2) we have for $\frac{p+1}{2} \leq j \leq p-2$ that

$$\begin{aligned} \Gamma_p\left(\frac{1}{2} + \frac{p+1}{2}\right)^2 &\equiv 1 \pmod{p} \\ \Gamma_p\left(\frac{1}{2} + \frac{p+1}{2} + 1\right)^2 &\equiv \left(\frac{p+2}{2}\right)^2 \pmod{p} \\ \Gamma_p\left(\frac{1}{2} + \frac{p+1}{2} + 2\right)^2 &\equiv \left(\frac{p+4}{2}\right)^2 \left(\frac{p+2}{2}\right)^2 \pmod{p} \\ &\vdots \\ \Gamma_p\left(\frac{1}{2} + p - 2\right)^2 &\equiv \left(\frac{2p-5}{2}\right)^2 \left(\frac{2p-7}{2}\right)^2 \cdots \left(\frac{p+2}{2}\right)^2 \pmod{p}. \end{aligned}$$

By Proposition 2.1 (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 $\frac{p+1}{2} \leq j \leq p-2$ and thus

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

This proves the result for $n = 1$. □

4. PROOF OF COROLLARY 1.2

Theorem 1.1 can be used to obtain modulo p^3 supercongruences in various settings. For example, Apéry numbers [3], traces of Frobenius endomorphisms on elliptic curves [24], [31], and colored partition functions [31] all occur as special values of ${}_{n+1}F_n(\lambda)$ for certain n and λ . We do not mention these results here, choosing instead to illustrate with one example. We now prove Corollary 1.2.

Proof. If p is an odd prime, then by Section 3 in [16],

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

and so by (8),

$$\left(\frac{-1}{p}\right) \equiv p^2 [X(p, 1, 1) + D(p, 1)] + pY(p, 1, 1) + Z(p, 1, 1) \pmod{p^3}.$$

We now claim that

$$(27) \quad X(p, 1, 1) + D(p, 1) + 1 \equiv 0 \pmod{p}.$$

In order to verify (27), we first study $X(p, 1, 1)$. By (3), we have

$$X(p, 1, 1) = \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2} + j}{j} \binom{\frac{p-1}{2}}{j} (-1)^j \left(1 + 4j \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right) + j^2 \left(2 \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right)^2 - \left(H_{\frac{p-1}{2}+j}^{(2)} - H_j^{(2)} \right) \right) \right).$$

The identity

$$(28) \quad \sum_{k=0}^n (-1)^k \binom{n+k}{k} \binom{n}{k} \left(1 + 2k \left(H_{n+k} - H_k \right) \right) = (-1)^n (2n+1)$$

was discovered using **Sigma** (see Lemma 2.2 in [27]). In particular, we find

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2} + j}{j} \binom{\frac{p-1}{2}}{j} (-1)^j \left(1 + 2j \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right) \right) \equiv 0 \pmod{p}$$

and thus

$$(29) \quad \begin{aligned} X(p, 1, 1) &\equiv -1 - \sum_{j=1}^{\frac{p-1}{2}} \binom{\frac{p-1}{2} + j}{j} \binom{\frac{p-1}{2}}{j} (-1)^j \\ &\quad + \sum_{j=1}^{\frac{p-1}{2}} \binom{\frac{p-1}{2} + j}{j} \binom{\frac{p-1}{2}}{j} (-1)^j \left(j^2 \left(2 \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right)^2 - \left(H_{\frac{p-1}{2}+j}^{(2)} - H_j^{(2)} \right) \right) \right) \pmod{p}. \end{aligned}$$

By Proposition 2.2 and Lemma 2.3, we also have

$$(30) \quad D(p, 1) \equiv \sum_{j=1}^{\frac{p-3}{2}} \binom{\frac{p-1}{2} + j}{j}^{-1} \binom{\frac{p-1}{2}}{j}^{-1} (-1)^j \pmod{p}.$$

For positive integers n , the relation

$$(31) \quad \begin{aligned} &\sum_{j=1}^n \binom{n+j}{j} \binom{n}{j} (-1)^j \left(j^2 \left(2 \left(H_{n+j}^{(1)} - H_j^{(1)} \right)^2 - \left(H_{n+j}^{(2)} - H_j^{(2)} \right) \right) \right) \\ &+ \sum_{j=1}^n \binom{n+j}{j}^{-1} \binom{n}{j}^{-1} (-1)^j = n(-1+2n)(-1)^n \end{aligned}$$

was found using **Sigma**. Equation (27) now follows upon taking $n = \frac{p-1}{2}$ in (31), in the identity

$$(32) \quad \sum_{j=1}^n \binom{n+j}{j} \binom{n}{j} (-1)^j = -1 + (-1)^n,$$

and reducing modulo p . We now consider $Y(p, 1, 1)$. By (4), we have

$$Y(p, 1, 1) = \sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}+j}{j} \binom{\frac{p-1}{2}}{j} (-1)^j \left(1 + j \left(H_{\frac{p-1}{2}+j}^{(1)} - H_j^{(1)} \right) + j \left(H_{\frac{p-1}{2}-j}^{(1)} - H_j^{(1)} \right) \right).$$

For positive integers n , the relation

$$(33) \quad \begin{aligned} & \sum_{j=0}^n \binom{n+j}{j} \binom{n}{j} (-1)^j \left(1 + j \left(H_{n+j}^{(1)} + H_{n-j}^{(1)} - 2H_j^{(1)} \right) \right) \\ &= (1+2n) \binom{2n}{n} (-1)^n - \frac{3}{2} n(1+n) (-1)^n \sum_{i=1}^n \frac{\binom{2i}{i}}{i} \end{aligned}$$

was discovered using **Sigma**. Taking $n = \frac{p-1}{2}$ in (33) and reducing mod p^2 , we have

$$(34) \quad Y(p, 1, 1) \equiv p + \frac{3}{8} (-1)^{\frac{p-1}{2}} \sum_{i=1}^{\frac{p-1}{2}} \binom{2i}{i} \frac{1}{i} \pmod{p^2}.$$

Equation (9) then follows from (5), (27), and (34). \square

5. FINDING AND PROVING IDENTITIES (31) AND (33) WITH **Sigma**

An efficient algorithm to find and prove identities involving nested definite and indefinite sum expressions, such as (31) and (33), has only recently been developed and implemented. Inspired by hypergeometric summation [34], in particular Zeilberger's creative telescoping method [42], and Karr's indefinite summation algorithm [19, 20] (extended to definite summations), the second author developed and implemented an algorithm using **Mathematica** to handle various summations. The resulting package is called **Sigma**. For a more detailed description of the algorithms incorporated into **Sigma**, please see [39]. Applications of this computer algebra package include proving identities that arise in the enumeration of rhombus tilings of a symmetric hexagon [12, 38], in the verification of Stembridge's totally symmetric plane partitions theorem [41, 6], and in certain Padé approximations [9]. In this section, we illustrate how the package can be used to discover and prove identities (31) and (33). For simplicity, we write H_k for $H_k^{(1)}$.

5.1. **Identity (33).** With `Sigma` we produce the following harmonic sum identities:

$$(35) \quad \sum_{k=0}^n (-1)^k \binom{n+k}{k} \binom{n}{k} k H_k = (-1)^n n(n+1)(2H_n - 1),$$

$$(36) \quad \sum_{k=0}^n (-1)^k \binom{n+k}{k} \binom{n}{k} k H_{n+k} = (-1)^n n(n+1)2H_n - (-1)^n n^2,$$

and

$$(37) \quad \sum_{k=0}^n (-1)^k \binom{n+k}{k} \binom{n}{k} k H_{n-k} = -(-1)^n (n+1)^2 + (-1)^n (2n+1) \binom{2n}{n} \\ + 2n(n+1)(-1)^n H_n - \frac{3}{2} n(n+1)(-1)^n \sum_{i=1}^n \frac{\binom{2i}{i}}{i}.$$

Then, combining (32), (36) and (37) we arrive at identity (33).

Remark 5.1. Note that (28), (35) and (36) can be proved using hypergeometric techniques which appear in [4] and [7]. The key observation is that differentiation of the rising factorial $(x)_k = x(x+1)\dots(x+k-1)$ (resp. $1/(x)_k$) in x and afterwards substituting $x = 1$ produces $(1)_k H_k$ (resp. $-H_k/(1)_k$). With this fact, one can produce, e.g., (35) by setting up the identity

$$(38) \quad \sum_{k=0}^n \frac{(-n)_k (n+1)_k}{k! (x)_k} k = -\frac{n(n+1)}{x} {}_2F_1(1-n, n+2; x+1; 1) = -\frac{n(n+1)}{x} \frac{(x-n-1)_{n-1}}{(x+1)_{n-1}}$$

with Gauss' theorem, differentiating (38) in x , and setting $x = 1$. Obviously, the successful application of this technique relies on the fact that one knows the underlying hypergeometric identity such as (38) for the particular case (35). It would be interesting to see proofs of identity (37), in particular of identity (31), along the lines sketched above. Recently, a skillful application of partial fraction decomposition has been used in [36] to derive identity (37), but so far no proof of identity (31) has been found.

Subsequently, we illustrate the computation steps for identity (37) which can be executed in a straightforward manner. 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]:= S = SigmaSum[SigmaPower[-1, k] k SigmaBinomial[n + k, k] \\ 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 5.2. 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]`

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

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

$$(39) \quad g(n, k+1) - g(n, k) = c_0(n)f(n, k) + c_1(n)f(n+1, k) + c_2(n)f(n+2, k)$$

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

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

delivered by **Sigma**. We verify (39) 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 (39) can be checked directly. Summing (39) 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]]`

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

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

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

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 $c_1 h_1(n) + c_2 h_2(n) + p(n)$ 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 (37):

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

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

Remark 5.3. Looking at the identities (32), (36) and (35) one immediately sees that the combination $(32) + 2 \cdot (36) - 2 \cdot (35)$ produces (28). Since the sums can be combined so nicely, we had also the hope to find a solution for the sum

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

`Sigma` was able to compute the recurrence

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

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

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

5.2. **Identity (31).** Finally, we derive the two identities

$$(40) \quad \sum_{k=1}^n \binom{n+k}{k} \binom{n}{k} (-1)^k \left(2k^2 (H_{n+k} - H_k)^2 - k^2 (H_{n+k}^{(2)} - H_k^{(2)}) \right) \\ = (1+n)^2 (-2 - 2n + n^2) \frac{(n!)^2 (-1)^n}{2(2+2n)!} + \frac{1}{4} n (-4 + 11n + 6n^2 + 3n^3) (-1)^n \\ - \frac{1}{2} (-1 + n + n^2) + \frac{3}{2} n^2 (1+n)^2 (-1)^n \sum_{i=1}^n \frac{i!^2}{(2+2i)!} + n^2 (1+n)^2 (-1)^n \sum_{i=1}^n \frac{(-1)^i}{i^2}$$

and

$$(41) \quad \sum_{k=1}^n \binom{n+k}{k}^{-1} \binom{n}{k}^{-1} (-1)^k = n(2n-1) (-1)^n \\ - \left((1+n)^2 (-2 - 2n + n^2) \frac{(n!)^2 (-1)^n}{2(2+2n)!} + \frac{1}{4} n (-4 + 11n + 6n^2 + 3n^3) (-1)^n \right. \\ \left. - \frac{1}{2} (-1 + n + n^2) + \frac{3}{2} n^2 (1+n)^2 (-1)^n \sum_{i=1}^n \frac{i!^2}{(2+2i)!} + n^2 (1+n)^2 (-1)^n \sum_{i=1}^n \frac{(-1)^i}{i^2} \right)$$

which immediately gives identity (31).

One option is to follow the same strategy as above: We can compute a recurrence for

$$\text{In}[6]:= \text{mySum} = \sum_{k=0}^n (-1)^k \binom{n+k}{k} \binom{n}{k} \left(2k^2 (H_{n+k} - H_k)^2 - k^2 (H_{n+k}^{(2)} - H_k^{(2)}) \right)$$

and can solve the derived recurrence to find the right hand side of (40). But, since the found recurrence relation is rather big (it has order 4), and the proof certificate is even bigger (it fills about one page), we follow a refined strategy presented in [33] and [40]. Namely, by running our creative telescoping algorithm with the additional option `SimplifyByExt` \rightarrow `DepthNumber` we can find a recurrence of smaller order (order one!):

$$\text{In}[7]:= \text{rec} = \text{GenerateRecurrence}[\text{mySum}, \text{SimplifyByExt} \rightarrow \text{DepthNumber}]$$

$$\text{Out}[7]= 2(2n+1)(n+2)^2 \text{SUM}[n] + 2(2n+1)n^2 \text{SUM}[n+1] == \\ 4(1+2n) + n^2(n+1)(n+2)(3n+2) \sum_{i=0}^n \frac{(-1)^i \binom{n+1}{i} \binom{n}{i}}{(n+i)^2} + 2n(4n^2+3n-4)(2n+1) \sum_{i=0}^n (-1)^i \binom{n+1}{i} \binom{n}{i} + \\ 8(n-1)n(n+1)(n+2)(2n+1) \left(\sum_{i=0}^n (-1)^i \binom{n+1}{i} \binom{n}{i} H_{n+i} - \sum_{i=0}^n (-1)^i \binom{n+1}{i} \binom{n}{i} H_i \right)$$

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

$$(42) \quad g(n, k+1) - g(n, k) = c_0(n) f(n, k) + c_1(n) f(n+1, k)$$

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

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

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

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

the verification of (42) is immediate. Summing (42) 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, facilitating again Sigma, we can produce mechanically the identities

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

and

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

Using in addition (32), we can simplify the recurrence to

$$\begin{aligned}
\text{In[8]:= rec} = & \text{rec} / \cdot \left\{ \sum_{i=0}^n (-1)^i \frac{\binom{n+i}{i} \binom{n}{i}}{(n+i)^2} \rightarrow -(-1)^n \frac{n!^2}{n^2(2n)!}, \sum_{i=0}^n (-1)^i \binom{n+i}{i} \binom{n}{i} \rightarrow (-1)^n, \right. \\
& \left. \sum_{i=0}^n (-1)^i \binom{n+i}{i} \binom{n}{i} H_i \rightarrow \sum_{i=0}^n (-1)^i \binom{n+i}{i} \binom{n}{i} H_{n+i} \right\}
\end{aligned}$$

$$\begin{aligned}
\text{Out[8]=} & 2(2n+1)n^2\text{SUM}[n+1] + 2(n+2)^2(2n+1)\text{SUM}[n] = \\
& 4(2n+1) - \frac{(-1)^n(n+1)(n+2)(3n+2)(n!)^2}{(2n)!} + 2(-1)^n n(2n+1)(4n^2+3n-4).
\end{aligned}$$

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

$$\text{In[9]:= recSol} = \text{SolveRecurrence[rec[[1]], SUM[n], SimpleSumRepresentation} \rightarrow \text{True]}$$

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

Looking at the first initial values we end up at the identity (40).

Finally, we attack the sum $S(n)$ on the left hand side of (41). Namely, we derive the recurrence

$$(n+2)S(n) + n^2 S(n) = \frac{(-1)^n (n+1)^2 (n+2)(3n+2)(n!)^2}{(2n+2)!} - 2;$$

we remark that for this hypergeometric sum any implementation of Zeilberger's algorithm [42] could do the job. Using this information, we find as above, the right hand side of (41).

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SCHOOL OF MATHEMATICAL SCIENCES, UNIVERSITY COLLEGE DUBLIN, BELFIELD, DUBLIN 4, IRELAND

IHÉS, LE BOIS-MARIE, 35, ROUTE DE CHARTRES, F-91440 BURES-SUR-YVETTE, FRANCE

RESEARCH INSTITUTE FOR SYMBOLIC COMPUTATION, J. KEPLER UNIVERSITY LINZ, ALTENBERGER STR. 69,
A-4040 LINZ, AUSTRIA

E-mail address: robert.osburn@ucd.ie, osburn@ihes.fr

E-mail address: Carsten.Schneider@risc.uni-linz.ac.at