ANNALES

DE

L'INSTITUT FOURIER

Robert OSBURN, Armin STRAUB & Wadim ZUDILIN

A modular supercongruence for ${}_6F_5$: An Apéry-like story

Tome 68, nº 5 (2018), p. 1987-2004.

<http://aif.cedram.org/item?id=AIF_2018__68_5_1987_0>

Ann. Inst. Fourier, Grenoble
68, 5 (2018) 1987-2004

A MODULAR SUPERCONGRUENCE FOR ${}_6F_5$: AN APÉRY-LIKE STORY

by Robert OSBURN, Armin STRAUB & Wadim ZUDILIN

Abstract. — We prove a supercongruence modulo p^3 between the pth Fourier coefficient of a weight 6 modular form and a truncated ${}_6F_5$-hypergeometric series. Novel ingredients in the proof are the comparison of two rational approximations to $\zeta(3)$ to produce non-trivial harmonic sum identities and the reduction of the resulting congruences between harmonic sums via a congruence relating the Apéry numbers to another Apéry-like sequence.

Résumé. — On démontre une supercongruence modulo p^3 entre le p-ième coefficient de Fourier d'une forme modulaire de poids 6 et une série hypergéométrique ${}_6F_5$ tronquée. Les nouveaux ingrédients de la preuve sont la comparaison de deux approximations rationnelles de $\zeta(3)$ pour produire des identités non triviales entre sommes harmoniques, et la réduction des congruences qui en résultent entre des sommes via une congruence qui relie les nombres d'Apéry á une autre suite du type de celle d'Apéry.

1. Introduction

There has been considerable recent interest in the study of arithmetic properties connecting pth Fourier coefficients of integral weight modular forms and truncated hypergeometric series. A motivating example of this phenomenon is the modular supercongruence [14]

$$(1.1)\qquad {}_4F_3\left[\begin{matrix}\frac12,\ \frac12,\ \frac12,\ \frac12\\ 1,\ 1,\ 1\end{matrix}\ \middle|\ 1\right]_{p-1} \equiv a(p) \pmod{p^3},$$

where p is an odd prime and $a(n)$ are the Fourier coefficients of the Hecke eigenform

$$(1.2)\qquad \eta(2\tau)^4\eta(4\tau)^4 = \sum_{n=1}^{\infty} a(n)q^n$$

Keywords: supercongruence, Apéry numbers, Apéry-like numbers, hypergeometric function.
2010 *Mathematics Subject Classification:* 11B65, 33C20, 33F10.

of weight 4 for the modular group $\Gamma_0(8)$. Here and throughout, $q = e^{2\pi i\tau}$ with $\operatorname{Im}\tau > 0$, $\eta(\tau) = q^{1/24}\prod_{n=1}^{\infty}(1-q^n)$ is Dedekind's eta function and

$$ {}_{n+1}F_n\left[\begin{matrix} a_0,\, a_1, \dots,\, a_n \\ b_1, \dots,\, b_n \end{matrix} \,\middle|\, z\right]_{p-1} = \sum_{k=0}^{p-1} \frac{(a_0)_k \cdots (a_n)_k}{(b_1)_k \cdots (b_n)_k} \frac{z^n}{n!}, $$

with $(a)_k = a(a+1)\cdots(a+k-1)$, is the truncated hypergeometric series.

Kilbourn's result (1.1) verifies one of 14 conjectural supercongruences between truncated ${}_4F_3$-hypergeometric series (evaluated at 1) corresponding to fundamental periods of the Picard–Fuchs differential equation for Calabi–Yau manifolds of dimension 3 and the Fourier coefficients of modular forms of weight 4 and varying level [26]. Two more cases have been proven in [10] and [18]. Moreover, there is now a general combinatorial framework [16, 17] which not only covers these 14 cases, but also the 8 cases in dimensions 1 and 2. In addition, (1.1) is one of van Hamme's original 13 Ramanujan-type supercongruences (see [12, (M.2)]). For further details on this and related topics we refer to [9, 13, 21, 29].

The purpose of this paper is to observe that a relationship akin to (1.1) exists between a truncated ${}_6F_5$-hypergeometric series and a modular form of weight 6. Our main result is the following.

Theorem 1.1. — *For all odd primes p,*

$$ {}_6F_5\left[\begin{matrix} \frac12,\, \frac12,\, \frac12,\, \frac12,\, \frac12,\, \frac12 \\ 1,\, 1,\, 1,\, 1,\, 1 \end{matrix} \,\middle|\, 1\right]_{p-1} \equiv b(p) \pmod{p^3}, \tag{1.3} $$

where

$$ \eta(\tau)^8\eta(4\tau)^4 + 8\eta(4\tau)^{12} = \eta(2\tau)^{12} + 32\eta(2\tau)^4\eta(8\tau)^8 = \sum_{n=1}^{\infty} b(n)q^n \tag{1.4} $$

is the unique newform in $S_6(\Gamma_0(8))$.

Theorem 1.1 is of particular practical relevance due to Weil's bounds $|b(p)| < 2p^{5/2}$, which tell us that the values of the truncated sums modulo p^3 are sufficient for reconstructing the Fourier coefficients $b(p)$, and hence the Hecke eigenform. Mortenson has further observed numerically that (1.3) appears to hold modulo p^5. The technical difficulties in generalizing our approach to verify this observation seem considerable. It would therefore be particularly interesting whether a different approach can be found, which verifies the congruence more naturally.

The paper is organized as follows. In §2, we provide additional historic context, going back to Apéry's proof of the irrationality of $\zeta(3)$, and introduce Apéry-like sequences. This also serves to prepare for our proof of

Theorem 1.1, which, interestingly, involves two constructions [19, 25, 31] of rational approximations to $\zeta(3)$ as well as a congruence between the Apéry numbers and another Apéry-like sequence. This congruence is proven in §3. In §4, we briefly review Greene's Gaussian hypergeometric series. A result of Frechette, Ono and Papanikolas [8] expresses the Fourier coefficients $b(p)$ in terms of these finite field analogs of the classical hypergeometric series. The Gaussian hypergeometric functions that thus arise have been determined modulo p^3 in [20] in terms of sums involving harmonic sums. In §5, we reduce the resulting congruences between sums involving harmonic numbers, then prove Theorem 1.1. One of the challenging auxiliary congruences is

$$\sum_{k=0}^{m}(-1)^k\binom{m+k}{k}^3\binom{m}{k}^3(1+3k(H_{m+k}+H_{m-k}-2H_k)) \equiv \sum_{k=0}^{m}\binom{m+k}{k}^2\binom{m}{k}^2 \pmod{p^2}. \tag{1.5}$$

Here, and throughout the paper, p is an odd prime and $m=(p-1)/2$. As usual, $H_n = H_n^{(1)}$, and $H_n^{(r)}$ denote the generalized harmonic numbers

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

The fact that the right-hand side of (1.5) involves the Apéry numbers and the relation of the latter to the irrationality of $\zeta(3)$ helped us to apply some "irrational" ingredients, in the form of two different constructions of rational approximations to $\zeta(3)$, to complete the proof. Finally, in §6, we comment on the need to certify congruences algorithmically.

Acknowledgments. The first and third authors would like to thank the organizers of the workshop "Modular forms in String Theory" (September 26–30, 2016) at the Banff International Research Station, Alberta (Canada). The three authors thank the Max Planck Institute for Mathematics in Bonn (Germany), where part of this research was performed. The third author would like to thank Ling Long for several helpful insights on links between finite and truncated hypergeometric functions.

2. Historic context and Apéry-like sequences

The Apéry numbers [28, A005259]

$$A(n)=\sum_{k=0}^{n}\binom{n}{k}^2\binom{n+k}{k}^2 \tag{2.1}$$

rose to prominence by Apéry's proof [2] of the irrationality of $\zeta(3)$ at the end of the 1970s and were studied by number theorists in the 1980s because of their arithmetic significance. Prominently, for instance, Beukers conceptualized Apéry's proof by realizing that the ordinary generating function admits a parametrization by modular forms. Beukers also established [4] a second relation to modular forms by showing that

$$A\left(\frac{p-1}{2}\right)\equiv a(p) \pmod{p}, \tag{2.2}$$

where $a(n)$ are the Fourier coefficients of the Hecke eigenform (1.2). After some dormancy, the Apéry numbers resurfaced when Ahlgren and Ono [1] proved Beukers' conjecture that (2.2) holds modulo p^2. In a different direction, Beukers and Zagier [30] initiated the exploration of generalizations, often referred to as Apéry-like sequences, which also arise as integral solutions to recurrence equations like

$$(n+1)^3A(n+1)-(2n+1)(17n^2+17n+5)A(n)+n^3A(n-1)=0, \tag{2.3}$$

which is satisfied by the Apéry numbers $A(n)$ and characterizes them together with the single initial condition $A(0)=1$.

In reducing the harmonic sums that we encounter in the proof of Theorem 1.1, a crucial role is played by the sequence $C_6(n)$, [28, A183204], where

$$C_\ell(n)=\sum_{k=0}^{n}\binom{n}{k}^\ell\bigl(1-\ell k(H_k-H_{n-k})\bigr). \tag{2.4}$$

The phenomenon that these sequences are integral for all positive integers ℓ has been proved in [15, Proposition 1]. For $\ell=1,2,3,4,5$, these sequences were explicitly evaluated by Paule and Schneider [22], who further ask whether $C_\ell(n)$ can be expressed as a single sum of hypergeometric terms for $\ell\geqslant 6$. It turns out that $C_6(n)$ is one of the sporadic Apéry-like sequences discovered in [7] (see also [32]), so that, for $\ell=6$, the question of Paule and Schneider is answered affirmatively by the following observation.

Proposition 2.1. — *The sequence $C_6(n)$ has the binomial sum representations*

$$C_6(n) = (-1)^n \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k} \binom{2k}{n}$$
$$= \sum_{k=0}^{n} (-1)^k \binom{3n+1}{n-k} \binom{n+k}{k}^3,$$

which make the integrality of $C_6(n)$ transparent.

That all three sums are equal can be verified by checking that each sequence satisfies the same three-term recursion (a variation of (2.3)). These are recorded in [22] and [7], or can be automatically derived by an algorithm such as creative telescoping. An expression for $C_6(n)$ as a variation of the first of the sums in Proposition 2.1, and hence the answer to the question of Paule and Schneider, for $\ell = 6$, was already observed in [6, Entry 17 in Table 2]. No single-sum hypergeometric expressions for $C_\ell(n)$ are known when $\ell \geqslant 7$.

The following unexpected congruence between the Apéry numbers $A(n)$ and the Apéry-like numbers $C_6(n)$, from (2.1) and (2.4), is another ingredient in our proof of Theorem 1.1. It is proved in §3.

Lemma 2.2. — *For all odd primes p,*

$$A\left(\frac{p-1}{2}\right) \equiv C_6\left(\frac{p-1}{2}\right) \pmod{p^2}. \tag{2.5}$$

We point out that suitable modular parameterizations of the generating functions $\sum_{n=0}^{\infty} A(n) z^n$ and $\sum_{n=0}^{\infty} C_6(n) z^n$ convert them into weight 2 modular forms of level 6 and 7, respectively [5] and [7]. We further note that the congruence (2.5) is rather trivially complemented by the congruence

$$A\left(\frac{p-1}{2}\right) \equiv D\left(\frac{p-1}{2}\right) \pmod{p},$$

which is straightforward and is only true modulo p, where

$$D(n) = \sum_{n=0}^{\infty} \binom{n}{k}^4$$

is another Apéry-like sequence [28, A005260], associated with a modular form of weight 2 and level 10 (see [7]).

3. Another Apéry number congruence

This section is concerned with proving the congruence (2.5) of Lemma 2.2 and, thereby, collecting some basic congruences involving harmonic numbers. The form in which we will later use this congruence is

$$\sum_{k=0}^{m}\binom{m}{k}^2\binom{m+k}{k}^2 \equiv \sum_{k=0}^{m}\binom{m}{k}^6\big(1-6k(H_k-H_{m-k})\big) \pmod{p^2}. \tag{3.1}$$

Here, and throughout, p is an odd prime and $m=(p-1)/2$. For our proof of the congruence (3.1) it is however crucial to use the alternative representation

$$C_6(n)=\sum_{k=0}^{n}(-1)^k\binom{3n+1}{n-k}\binom{n+k}{k}^3$$

for the sequence $C_6(n)$ provided by Proposition 2.1.

First, note that

$$\binom{m+k}{m}=\frac{(m+1)_k}{k!}=\frac{(\frac{1}{2})_k}{k!}\left(1+\frac{p}{2}\sum_{j=0}^{k-1}\frac{1}{j+\frac{1}{2}}+O(p^2)\right) \tag{3.2}$$

and

$$\binom{m}{k}=\frac{(-1)^k(-m)_k}{k!}=(-1)^k\,\frac{(\frac{1}{2})_k}{k!}\left(1-\frac{p}{2}\sum_{j=0}^{k-1}\frac{1}{j+\frac{1}{2}}+O(p^2)\right). \tag{3.3}$$

Now, since

$$\begin{aligned}\sum_{j=0}^{k-1}\frac{1}{j+\frac{1}{2}}&=\sum_{j=0}^{k-1}\frac{1}{j+\frac{1}{2}+\frac{p}{2}}+O(p)=\sum_{j=0}^{k-1}\frac{1}{j+m+1}+O(p)\\&=H_{m+k}-H_m+O(p),\end{aligned}$$

we can write the expressions (3.2) and (3.3) in the forms

$$\binom{m}{k}=(-1)^k\,\frac{(\frac{1}{2})_k}{k!}\left(1-\frac{p}{2}(H_{m+k}-H_m)+O(p^2)\right), \tag{3.4}$$

and

$$\begin{aligned}\binom{m+k}{m}&=\frac{(\frac{1}{2})_k}{k!}\left(1+\frac{p}{2}(H_{m+k}-H_m)+O(p^2)\right)\\&=(-1)^k\binom{m}{k}\left(1+\frac{p}{2}(H_{m+k}-H_m)+O(p^2)\right)^2\\&=(-1)^k\binom{m}{k}\big(1+p(H_{m+k}-H_m)+O(p^2)\big).\end{aligned} \tag{3.5}$$

Recall that $2m = p-1$, so that

$$H_{2m-k} = H_{p-1} - \sum_{j=1}^{k} \frac{1}{p-j} = \sum_{j=1}^{k} \left(\frac{1}{j} + \frac{p}{j^2} \right) + O(p^2) \tag{3.6}$$
$$= H_k + pH_k^{(2)} + O(p^2).$$

By swapping k with $m-k$, we get

$$H_{m+k} = H_{m-k} + pH_{m-k}^{(2)} + O(p^2), \tag{3.7}$$

and, in view of the invariance of $\binom{m}{k}$ under replacing k with $m-k$, we can translate formula (3.5) to

$$\binom{2m-k}{m} = (-1)^{m-k} \binom{m}{k} \big(1 + p(H_{2m-k} - H_m) + O(p^2)\big) \tag{3.8}$$
$$= (-1)^{m-k} \binom{m}{k} \big(1 + p(H_k - H_m) + O(p^2)\big),$$

which will be useful later.

On the other hand,

$$\binom{3m+1}{k} = \binom{m+p}{k} = (-1)^k \frac{(-m-p)_k}{k!}$$
$$= (-1)^k \frac{(-m)_k}{k!} \left(1 - p \sum_{j=0}^{k-1} \frac{1}{-m-p+j} + O(p^2) \right)$$
$$= \binom{m}{k} \big(1 + p(H_m - H_{m-k}) + O(p^2)\big),$$

so that

$$\binom{3m+1}{m-k} = \binom{m}{k} \big(1 + p(H_m - H_k) + O(p^2)\big). \tag{3.9}$$

It follows from (3.5), (3.7) and (3.9) that

$$\binom{m+k}{m}^2 \binom{m}{k}^2 = \binom{m}{k}^4 \big(1 + p(H_{m-k} - H_m) + O(p^2)\big)^2$$
$$= \binom{m}{k}^4 \big(1 + p(2H_{m-k} - 2H_m) + O(p^2)\big)$$

and

$$\begin{aligned}
(-1)^k &\binom{3m+1}{m-k}\binom{m+k}{m}^3 \\
&= \binom{m}{k}^4 \big(1+p(H_m-H_k)+O(p^2)\big)\big(1+p(H_{m-k}-H_m)+O(p^2)\big)^3 \\
&= \binom{m}{k}^4 \big(1+p(3H_{m-k}-H_k-2H_m)+O(p^2)\big).
\end{aligned}$$

It remains to use the symmetry $k \leftrightarrow m-k$ in the form

$$\sum_{k=0}^{m} \binom{m}{k}^4 H_{m-k} = \sum_{k=0}^{m} \binom{m}{k}^4 H_k$$

to conclude that the desired congruence (2.5) is indeed true modulo p^2.

4. Gaussian hypergeometric series

In the following, we discuss some preliminaries concerning Greene's Gaussian hypergeometric series [11]. Let $\mathbb{F}_p$ denote the finite field with p elements. We extend the domain of all characters χ of $\mathbb{F}_p^\times$ to $\mathbb{F}_p$ by defining $\chi(0)=0$. For characters A and B of $\mathbb{F}_p^\times$, define

$$\binom{A}{B} = \frac{B(-1)}{p} J(A,\bar{B}),$$

where $J(\chi,\lambda)$ denotes the Jacobi sum for χ and λ characters of $\mathbb{F}_p^\times$. For characters $A_0, A_1, \dots, A_n$ and $B_1, \dots, B_n$ of $\mathbb{F}_p^\times$ and $x \in \mathbb{F}_p$, define the Gaussian hypergeometric series by

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

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

We consider the case where $A_i = \phi_p$, the quadratic character, for all i, and $B_j = \epsilon_p$, the trivial character mod p, for all j, and write

$${}_{n+1}F_n(x) = {}_{n+1}F_n\left(\begin{matrix} \phi_p,\, \phi_p,\, \dots,\, \phi_p \\ \epsilon_p,\, \dots,\, \epsilon_p \end{matrix} \,\middle|\, x\right)_p$$

for brevity. By [11], $p^n\,{}_{n+1}F_n(x) \in \mathbb{Z}$.

For $\lambda \in \mathbb{F}_p$ and $\ell \geqslant 2$ an integer, we now define the quantities

$$X_\ell(p,\lambda) = \lambda^m \sum_{k=0}^{m} (-1)^{\ell k} \binom{m+k}{k}^\ell \binom{m}{k}^\ell \Big(1 + 4\ell k (H_{m+k} - H_k) + 2\ell^2 k^2 (H_{m+k} - H_k)^2 - \ell k^2 \Big(H^{(2)}_{m+k} - H^{(2)}_k\Big)\Big)\lambda^{-k},$$

$$Y_\ell(p,\lambda) = \lambda^m \sum_{k=0}^{m} (-1)^{\ell k} \binom{m+k}{k}^\ell \binom{m}{k}^\ell \big(1 + 2\ell k (H_{m+k} - H_k) - \ell k (H_{m+k} - H_{m-k})\big)\lambda^{-kp},$$

$$Z_\ell(p,\lambda) = \lambda^m \sum_{k=0}^{m} \binom{2k}{k}^{2\ell} 16^{-\ell k} \lambda^{-kp^2}.$$

Here, as before, $m = (p-1)/2$.

The main result in [20] provides an expression for ${}_{2\ell}F_{2\ell-1}$ modulo p^3. Precisely, we have the following.

Theorem 4.1. — *Let p be an odd prime, $\lambda \in \mathbb{F}_p$, and $\ell \geqslant 2$ be an integer. Then*

$$p^{2\ell-1}{}_{2\ell}F_{2\ell-1}(\lambda) \equiv -\big(p^2 X_\ell(p,\lambda) + pY_\ell(p,\lambda) + Z_\ell(p,\lambda)\big) \pmod{p^3}.$$

An analogous result holds for the opposite parity, that is, for ${}_{n+1}F_n$ when n is even.

5. Two lemmas and the proof of Theorem 1.1

Lemma 5.1. — *Let p be an odd prime. Then*

$$X_3(p,1) - Y_2(p,1) \equiv (-1)^{(p-1)/2} - 1 \pmod{p}.$$

Proof. — Consider the rational function

$$R(t) = R_n(t) = \frac{\prod_{j=1}^{n}(t-j)^2}{\prod_{j=0}^{n}(t+j)^2},$$

defined for any integer $n \geqslant 0$. Its partial fraction decomposition assumes the form

$$R(t) = \sum_{k=0}^{n} \left(\frac{A_k}{(t+k)^2} + \frac{B_k}{t+k}\right),$$

where

$$A_k = \big(R(t)(t+k)^2\big)\big|_{t=-k} = \binom{n+k}{k}^2 \binom{n}{k}^2,$$

and, on considering the logarithmic derivative of $R(t)(t+k)^2$,

$$\begin{aligned}
B_k &= \frac{\mathrm{d}}{\mathrm{d}t}\big(R(t)(t+k)^2\big)\Big|_{t=-k} \\
&= 2\big(R(t)(t+k)^2\big)\Bigg(\sum_{j=1}^{n}\frac{1}{t-j} - \sum_{\substack{j=0\\ j\neq k}}^{n}\frac{1}{t+j}\Bigg)\Bigg|_{t=-k} \\
&= 2A_k\,\big((H_k - H_{n+k}) + (H_k - H_{n-k})\big).
\end{aligned}$$

The related partial fraction decomposition

$$\begin{aligned}
tR(t) &= \sum_{k=0}^{n}\left(\frac{A_k t}{(t+k)^2} + \frac{B_k t}{t+k}\right) \\
&= \sum_{k=0}^{n}\left(\frac{A_k((t+k)-k)}{(t+k)^2} + \frac{B_k((t+k)-k)}{t+k}\right) \\
&= \sum_{k=0}^{n}\left(-\frac{kA_k}{(t+k)^2} + \frac{A_k - kB_k}{t+k} + B_k\right)
\end{aligned}$$

and the residue sum theorem imply

$$\begin{aligned}
\sum_{k=0}^{n}(A_k - kB_k) &= \sum_{\text{all finite poles}} \operatorname{Res}_{\text{pole}} tR(t) = -\operatorname{Res}_{t=\infty} tR(t) \\
&= \text{coefficient of } s \text{ in Taylor's } s\text{-expansion of } \frac{1}{s}\,R\Big(\frac{1}{s}\Big) \\
&= \text{coefficient of } s \text{ in Taylor's } s\text{-expansion of } s\,\frac{\prod_{j=1}^{m}(1-js)^2}{\prod_{j=0}^{m}(1+js)^2} \\
&= 1 = A_0,
\end{aligned}$$

from which $\sum_{k=1}^{n}(A_k - kB_k) = 0$ follows. The resulting identity is then

$$\sum_{k=0}^{n}\binom{n+k}{k}^2\binom{n}{k}^2\big(1 - 2k(2H_k - H_{n+k} - H_{n-k})\big) = 1, \tag{5.1}$$

which played a crucial role in [1] and [14]. Notice that (5.1) implies

$$Y_2(p,1) = 1. \tag{5.2}$$

Equality (5.1) and its derivation above follow the approach of Nesterenko from [19] of proving Apéry's theorem (see also [31]).

We can perform a similar analysis for the rational function

$$\widetilde{R}(t) = \widetilde{R}_n(t) = \frac{\prod_{j=1}^{n}(t-j)^3}{\prod_{j=0}^{n}(t+j)^3} = \sum_{k=0}^{n}\left(\frac{\widetilde{A}_k}{(t+k)^3} + \frac{\widetilde{B}_k}{(t+k)^2} + \frac{\widetilde{C}_k}{t+k}\right).$$

As before, we get

$$\begin{aligned}
\widetilde{A}_k &= \left(\widetilde{R}(t)(t+k)^3\right)\Big|_{t=-k} = (-1)^{n+k}\binom{n+k}{k}^3\binom{n}{k}^3,\\
\widetilde{B}_k &= 3\widetilde{A}_k\,(2H_k - H_{n+k} - H_{n-k}),\\
\widetilde{C}_k &= \frac{9}{2}\widetilde{A}_k\,(2H_k - H_{n+k} - H_{n-k})^2 - \frac{3}{2}\widetilde{A}_k\left(H_{n+k}^{(2)} - 2H_k^{(2)} - H_{n-k}^{(2)}\right)
\end{aligned}$$

and by considering the sum of the residues of the rational functions $R(t)$, $tR(t)$ and $t^2R(t)$, we deduce that

$$\sum_{k=0}^{n}\widetilde{C}_k = \sum_{k=0}^{n}(\widetilde{B}_k - k\widetilde{C}_k) = 0 \qquad \text{and} \qquad \sum_{k=0}^{n}(\widetilde{A}_k - 2k\widetilde{B}_k + k^2\widetilde{C}_k) = 1.$$

We only record the first and last equalities for our future use:

$$\begin{aligned}
\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}^3\binom{n}{k}^3\Big(&3(2H_k - H_{n+k} - H_{n-k})^2\\
&- \left(H_{n+k}^{(2)} - 2H_k^{(2)} - H_{n-k}^{(2)}\right)\Big) = 0
\end{aligned} \tag{5.3}$$

and

$$\begin{aligned}
\sum_{k=0}^{n}(-1)^k\binom{n+k}{k}^3\binom{n}{k}^3\Big(&1 - 6k(2H_k - H_{n+k} - H_{n-k})\\
+\frac{9}{2}k^2(2H_k - H_{n+k} - H_{n-k})^2 &- \frac{3}{2}k^2\left(H_{n+k}^{(2)} - 2H_k^{(2)} - H_{n-k}^{(2)}\right)\Big) = (-1)^n.
\end{aligned} \tag{5.4}$$

Recall that, throughout, $m = (p-1)/2$. Now, taking $n = m$ in (5.4) and applying $H_{m-k} \equiv H_{m+k} \pmod p$ and $H_{m-k}^{(2)} \equiv -H_{m+k}^{(2)} \pmod p$, we obtain

$$\begin{aligned}
X_3(p,1) = \sum_{k=0}^{m}(-1)^k\binom{m+k}{k}^3\binom{m}{k}^3\Big(&1 - 12k(H_k - H_{m+k})\\
&+ 18k^2(H_k - H_{m+k})^2 - 3k^2\left(H_{m+k}^{(2)} - H_k^{(2)}\right)\Big)\\
\equiv (-1)^m \pmod p.&
\end{aligned} \tag{5.5}$$

The result then follows after combining (5.2) with (5.5). □

Lemma 5.2. — *Let p be an odd prime. Then*

$$Y_3(p,1) \equiv Z_2(p,1) \pmod{p^2}.$$

Proof. — Consider the rational function

$$\widehat{R}(t)=\widehat{R}_n(t)=\frac{n!^2\,(2t+n)\prod_{j=1}^{n}(t-j)\cdot\prod_{j=1}^{n}(t+n+j)}{\prod_{j=0}^{n}(t+j)^4}$$
$$=\sum_{k=0}^{n}\biggl(\frac{\widehat{A}_k}{(t+k)^4}+\frac{\widehat{B}_k}{(t+k)^3}+\frac{\widehat{C}_k}{(t+k)^2}+\frac{\widehat{D}_k}{t+k}\biggr).$$

Then

$$\widehat{A}_k=(-1)^n((n-k)-k)\binom{n+k}{n}\binom{2n-k}{n}\binom{n}{k}^4,$$
$$\widehat{B}_k=(-1)^n\binom{n+k}{n}\binom{2n-k}{n}\binom{n}{k}^4\bigl(2+(n-2k)\bigl(-(H_{n+k}-H_k)$$
$$+(H_{2n-k}-H_{n-k})-4(H_{n-k}-H_k)\bigr)\bigr).$$

An important consequence of a hypergeometric transformation due to W. N. Bailey [3], [33] (see also [25] and [31] for the links with rational approximations to $\zeta(3)$) is the equality

$$A(n)=\frac{1}{2}\sum_{k=0}^{n}\widehat{B}_k=\frac{(-1)^n}{2}\sum_{k=0}^{n}\binom{n+k}{n}\binom{2n-k}{n}\binom{n}{k}^4$$
$$\times(2+(n-2k)(5H_k-5H_{n-k}-H_{n+k}+H_{2n-k})). \tag{5.6}$$

Now, take $n=m$ (recall that $m=(p-1)/2$) and let $b(m,k)$ denote the summand in (5.6). Note that $b(m,k)=b(m,m-k)$ and substituting of (3.5) and (3.8) implies that

$$b(m,k) \tag{5.7}$$
$$=\binom{m}{k}^6\bigl(1+p(H_{m+k}-H_m)+O(p^2)\bigr)$$
$$\times\bigl(1+p(H_k-H_m)+O(p^2)\bigr)$$
$$\times\bigl(2+(m-2k)(5H_k-5H_{m-k}-H_{m+k}+H_{2m-k})\bigr)$$
$$=\binom{m}{k}^6\bigl(1+p(H_k+H_{m-k}-2H_m)+O(p^2)\bigr)$$
$$\times\Bigl(2+(m-2k)\Bigl(6H_k-6H_{m-k}+pH_k^{(2)}-pH_{m-k}^{(2)}+O(p^2)\Bigr)\Bigr)$$
$$=\binom{m}{k}^6\Bigl(2+6(m-2k)(H_k-H_{m-k})+2p(H_k+H_{m-k}-2H_m)$$
$$+6p(m-2k)(H_k^2-H_{m-k}^2)-12p(m-2k)(H_k-H_{m-k})H_m$$
$$+p(m-2k)\Bigl(H_k^{(2)}-H_{m-k}^{(2)}\Bigr)+O(p^2)\Bigr).$$

Moreover, it follows from the symmetry $k \leftrightarrow m-k$ in the form

$$\sum_{k=0}^{m} \binom{m}{k}^6 H_m = \sum_{k=0}^{m} \binom{m}{k}^6 H_{m-k}$$

as well as Lemma 2.2, (3.1) and (5.6) that

$$\begin{aligned}\sum_{k=0}^{m} \binom{m}{k}^6 \big(1+3(m-2k)(H_k-H_{m-k})\big) \\ = \sum_{k=0}^{m} \binom{m}{k}^6 \big(1-6k(H_k-H_{m-k})\big) \equiv \frac{1}{2}\sum_{k=0}^{m} b(m,k) \pmod{p^2}.\end{aligned}$$

Substitution of the expansion (5.7) into the latter congruence results, after simplifications, in

$$\begin{aligned}\sum_{k=0}^{m} \binom{m}{k}^6 \Big(2(H_k+H_{m-k}-2H_m)+6(m-2k)(H_k^2-H_{m-k}^2) \\ -12(m-2k)(H_k-H_{m-k})H_m \\ +(m-2k)\Big(H_k^{(2)}-H_{m-k}^{(2)}\Big)\Big) \equiv 0 \pmod{p}.\end{aligned} \tag{5.8}$$

From a different source, namely, from the equality (5.3) applied with $n=m$ and reduced modulo p, we obtain

$$\sum_{k=0}^{m} \binom{m}{k}^6 \Big(6(H_k-H_{m-k})^2+\Big(H_k^{(2)}+H_{m-k}^{(2)}\Big)\Big) \equiv 0 \pmod{p}. \tag{5.9}$$

Furthermore, denote

$$c(m,k) = (-1)^k \binom{m+k}{k}^3 \binom{m}{k}^3 \big(1+3k(H_{m+k}+H_{m-k}-2H_k)\big),$$

the summand of $Y_3(p,1)$. Then, with the help of (3.5), we obtain

$$\begin{aligned}c(m,k) &= \binom{m}{k}^6 \big(1+p(H_{m+k}-H_m)+O(p^2)\big)^3 \\ &\quad \times \big(1+3k(H_{m+k}+H_{m-k}-2H_k)\big) \\ &= \binom{m}{k}^6 \Big(1-6k(H_k-H_{m-k})+3p(H_{m-k}-H_m) \\ &\quad -18pk(H_k-H_{m-k})(H_{m-k}-H_m)+3pkH_{m-k}^{(2)}+O(p^2)\Big)\end{aligned}$$

and thus

$$\sum_{k=0}^{m} c(m,k) = \sum_{k=0}^{m} \widetilde{c}(m,k), \tag{5.10}$$

where

$$
\begin{aligned}
(5.11)\quad \widetilde{c}(m,k) &= \frac{c(m,k)+c(m,m-k)}{2} \\
&= \binom{m}{k}^6 \Big(1+3(m-2k)(H_k-H_{m-k}) \\
&\quad + \frac{3}{2}p(H_k+H_{m-k}-2H_m) - 9pmH_kH_{m-k} \\
&\quad - 9p(m-2k)(H_k-H_{m-k})H_m + 9p(m-k)H_k^2 \\
&\quad + 9pkH_{m-k}^2 + \frac{3}{2}p(m-k)H_k^{(2)} + \frac{3}{2}pkH_{m-k}^{(2)} + O(p^2)\Big).
\end{aligned}
$$

Finally, from (3.2) and (3.3), we have

$$\binom{2k}{k}^2 2^{-4k} = \frac{(1/2)_k^2}{k!^2} \equiv (-1)^k \binom{m+k}{m}\binom{m}{k} \pmod{p^2},$$

and so

$$Z_2(p,1) \equiv A(m) \pmod{p^2}. \tag{5.12}$$

Therefore, by (5.6), (5.7) and (5.10)–(5.12),

$$
\begin{aligned}
Y_3(p,1) - Z_2(p,1) &= \sum_{k=0}^{m} c(m,k) - \frac{1}{2}\sum_{k=0}^{m} b(m,k) \\
&= \frac{p}{2}\sum_{k=0}^{m}\binom{m}{k}^6 \Big((H_k+H_{m-k}-2H_m) - 18mH_kH_{m-k} \\
&\quad - 6(m-2k)(H_k-H_{m-k})H_m + (2m-k)\big(6H_k^2+H_k^{(2)}\big) \\
&\quad + (m+k)\big(6H_{m-k}^2 + H_{m-k}^{(2)}\big)\Big) + O(p^2).
\end{aligned}
$$

The latter sum is seen to be half of the sum in (5.8) plus $\frac{3}{2}m$ times the sum in (5.9). Thus, the result follows. □

We now prove our main result.

Proof of Theorem 1.1. — It was conjectured by Koike and proven by Frechette, Ono and Papanikolas that the Fourier coefficients $b(p)$ of (1.4) can be represented in terms of Gaussian hypergeometric series. Specifically, we have (see [8, Corollary 1.6])

$$b(p) = -p^5 {}_6F_5(1) + p^4 {}_4F_3(1) + \big(1-\phi_p(-1)\big)p^2.$$

We now apply Theorem 4.1 with $\ell = 2$ and $\ell = 3$, respectively, and simplify to obtain

$$b(p) \equiv p^2\big(X_3(p,1) - Y_2(p,1) + 1 - (-1)^{(p-1)/2}\big) \\ + p\big(Y_3(p,1) - Z_2(p,1)\big) + Z_3(p,1) \pmod{p^3}.$$

As

$$Z_3(p,1) = \sum_{n=0}^{(p-1)/2} \frac{(1/2)_n^6}{n!^6} \equiv \sum_{n=0}^{p-1} \frac{(1/2)_n^6}{n!^6} \pmod{p^6},$$

since the summands for $(p-1)/2 < n \leqslant p-1$ are divisible by p^6, the result follows from Lemmas 5.1 and 5.2. □

6. $A \equiv B$ wanted

At the time of Apéry's proof it was by no means trivial to verify identities $A = B$ like the ones in Proposition 2.1 by verifying that both sides, A and B, satisfy the same recurrence. For instance, van der Poorten's beautiful article [24] describes the difficulty in checking Apéry's claim that the Apéry numbers $A(n)$ satisfy the recurrence (2.3), and principally attributes to Cohen and Zagier the clever insight to prove the claim using creative telescoping. Since then, Wilf and Zeilberger, with subsequent support by many others, have developed creative telescoping into a pillar of a rich computer algebraic theory devoted to automatically proving identities between, for instance, holonomic functions and sequences. We refer to [23] for a superb introduction to these ideas. Among the more recent developments is Schneider's work [27], which extends the scope from holonomic sequences to a class of sequences that also includes nested sums of terms involving harmonic numbers. For instance, using Schneider's computer algebra package SIGMA, it is routine to verify that, for all integers $n \geqslant 0$,

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

which we derived earlier as (5.1) and which played a crucial role in Ahlgren and Ono's proof [1] of Beuker's conjecture as well as Kilbourn's proof [14] of the supercongruence (1.1).

Building on these ideas, proving our main result (1.3) modulo p^2, instead of p^3, is much more straightforward as this corresponds to verifying Lemma 5.2 modulo p only, a task that can be performed in many different ways (for example, using Kilbourn's strategy from [14, §4]). Working modulo higher powers of p is considerably more difficult. In the course of the derivation of Theorem 1.1 we encountered several technical difficulties that were finally resolved by an intelligent cast of hypergeometric identities. Specifically, in order to compute the congruence (1.3) we required the identities of Proposition 2.1 as well as the equalities (5.1), (5.3), (5.4) and (5.6), reduced modulo a suitable power of p. Note that all these *identities* can, nowadays, be easily resolved by using computer algebraic techniques like the algorithms from [23] and [27] mentioned above. We are, however, very restricted in this production because certain *congruences* (are expected to) remain not derivable this way. For example, establishing (1.3) modulo p^5 (or even p^4) by using appropriate intermediate identities sounds to us like a real challenge!

There is therefore a natural need for an algorithmic approach to directly certifying congruences $A \equiv B$, say, when the terms A and B are holonomic. Specifically, it would be great if such an approach could handle congruences such as (1.5), or even just (2.5) in the form

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

where $n = (p-1)/2$ and p is an odd prime.

BIBLIOGRAPHY

[1] S. Ahlgren & K. Ono, "A Gaussian hypergeometric series evaluation and Apéry number congruences", *J. Reine Angew. Math.* **518** (2000), p. 187-212.

[2] R. Apéry, "Irrationalité de $\zeta(2)$ et $\zeta(3)$", Astérisque, vol. 61, Société Mathématique de France, 1979, p. 11-13.

[3] W. N. Bailey, *Generalized hypergeometric series*, Cambridge Tracts in Mathematics and Mathematical Physics, vol. 32, Stechert-Hafner, 1964, v+108 pages.

[4] F. Beukers, "Another congruence for the Apéry numbers", *J. Number Theory* **25** (1987), no. 2, p. 201-210.

[5] ———, "Irrationality proofs using modular forms", in *Journées arithmétiques de Besançon (Besançon, 1985)*, Astérisque, vol. 147-148, Société Mathématique de France, 1987, p. 271-283.

[6] W. Chu & L. De Donno, "Hypergeometric series and harmonic number identities", *Adv. Appl. Math.* **34** (2005), no. 1, p. 123-137.

[7] S. Cooper, "Sporadic sequences, modular forms and new series for $1/\pi$", *Ramanujan J.* **29** (2012), no. 1-3, p. 163-183.

[8] S. Frechette, K. Ono & M. Papanikolas, "Gaussian hypergeometric functions and traces of Hecke operators", *Int. Math. Res. Not.* **2004** (2004), no. 60, p. 3233-3262.

[9] J. G. Fuselier, L. Long, R. Ramakrishna, H. Swisher & F.-T. Tu, "Hypergeometric functions over finite fields", `http://arxiv.org/abs/1510.02575`, 2015.

[10] J. G. Fuselier & D. McCarthy, "Hypergeometric type identities in the p-adic setting and modular forms", *Proc. Am. Math. Soc.* **144** (2016), no. 4, p. 1493-1508.

[11] J. Greene, "Hypergeometric functions over finite fields", *Trans. Am. Math. Soc.* **301** (1987), no. 1, p. 77-101.

[12] L. van Hamme, "Some conjectures concerning partial sums of generalized hypergeometric series", in *p-adic functional analysis (Nijmegen, 1996)*, Lecture Notes in Pure and Appl. Math., vol. 192, Dekker, 1997, p. 223-236.

[13] J. Kibelbek, L. Long, K. Moss, B. Sheller & H. Yuan, "Supercongruences and complex multiplication", *J. Number Theory* **164** (2016), p. 166-178.

[14] T. Kilbourn, "An extension of the Apéry number supercongruence", *Acta Arith.* **123** (2006), no. 4, p. 335-348.

[15] C. Krattenthaler & T. Rivoal, "Hypergéométrie et fonction zêta de Riemann", *Mem. Am. Math. Soc.* **186** (2007), no. 875, p. x+87.

[16] D. McCarthy, "Binomial coefficient-harmonic sum identities associated to supercongruences", *Integers* **11** (2011), Art A37, 8 p.

[17] ———, "Extending Gaussian hypergeometric series to the p-adic setting", *Int. J. Number Theory* **8** (2012), no. 7, p. 1581-1612.

[18] ———, "On a supercongruence conjecture of Rodriguez-Villegas", *Proc. Am. Math. Soc.* **140** (2012), no. 7, p. 2241-2254.

[19] Yu. V. Nesterenko, "Some remarks on $\zeta(3)$", *Mat. Zametki* **59** (1996), no. 6, p. 865-880.

[20] R. Osburn & C. Schneider, "Gaussian hypergeometric series and supercongruences", *Math. Comput.* **78** (2009), no. 265, p. 275-292.

[21] R. Osburn & W. Zudilin, "On the (K.2) supercongruence of Van Hamme", *J. Math. Anal. Appl.* **433** (2016), no. 1, p. 706-711.

[22] P. Paule & C. Schneider, "Computer proofs of a new family of harmonic number identities", *Adv. Appl. Math.* **31** (2003), no. 2, p. 359-378.

[23] M. Petkovšek, H. S. Wilf & D. Zeilberger, $A = B$, Peters, 1996, With a foreword by Donald E. Knuth, With a separately available computer disk, xii+212 pages.

[24] A. van der Poorten, "A proof that Euler missed: Apéry's proof of the irrationality of $\zeta(3)$", *Math. Intell.* **1** (1979), no. 4, p. 195-203.

[25] T. Rivoal, "Propriétés diophantinnes des valeurs de la fonction zêta de Riemann aux entiers impairs", PhD Thesis, Université de Caen (France), 2001.

[26] F. Rodriguez-Villegas, "Hypergeometric families of Calabi–Yau manifolds", in *Calabi–Yau varieties and mirror symmetry (Toronto, ON, 2001)*, Fields Inst. Commun., vol. 38, American Mathematical Society, 2003, p. 223-231.

[27] C. Schneider, "Symbolic summation assists combinatorics", *Sémin. Lothar. Comb.* **56** (2007), Art. B56b, 36 p.

[28] N. J. A. Sloane, "The On-Line Encyclopedia of Integer Sequences", 2017, published electronically at `http://oeis.org`.

[29] H. Swisher, "On the supercongruence conjectures of van Hamme", *Res. Math. Sci.* **2** (2015), Art. 18, 21 p.

[30] D. Zagier, "Integral solutions of Apéry-like recurrence equations", in *Groups and symmetries*, CRM Proc. Lecture Notes, vol. 47, American Mathematical Society, 2009, p. 349-366.

[31] W. Zudilin, "Apéry's theorem. Thirty years after", *Int. J. Math. Comput. Sci.* **4** (2009), no. 1, p. 9-19.

[32] ———, "A generating function of the squares of Legendre polynomials", *Bull. Aust. Math. Soc.* **89** (2014), no. 1, p. 125-131.

[33] ———, "Hypergeometric heritage of W. N. Bailey. With an appendix: Bailey's letters to F. Dyson", `http://arxiv.org/abs/1611.08806`, 2016.

Manuscrit reçu le 6 février 2017,
accepté le 14 novembre 2017.

Robert OSBURN
School of Mathematics and Statistics
University College Dublin
Belfield, Dublin 4 (Ireland)
robert.osburn@ucd.ie

Armin STRAUB
Dept. of Mathematics and Statistics
University of South Alabama
411 University Blvd N
MSPB 325, Mobile, AL 36688 (USA)
straub@southalabama.edu

Wadim ZUDILIN
Dept. of Mathematics, IMAPP
Radboud Universiteit
PO Box 9010
6500 GL Nijmegen (Netherlands)
and
School of Math. and Phys. Sciences
The University of Newcastle
Callaghan, NSW 2308 (Australia)
w.zudilin@math.ru.nl