

# LUCAS CONGRUENCES FOR THE APÉRY NUMBERS MODULO $p^2$

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ABSTRACT. The sequence  $A(n)_{n \geq 0}$  of Apéry numbers can be interpolated to  $\mathbb{C}$  by an entire function. We give a formula for the Taylor coefficients of this function, centered at the origin, as a  $\mathbb{Z}$ -linear combination of multiple zeta values. We then show that for integers  $n$  whose base- $p$  digits belong to a certain set,  $A(n)$  satisfies a Lucas congruence modulo  $p^2$ .

## 1. INTRODUCTION

For each integer  $n \geq 0$ , the  $n$ th *Apéry number* is defined by

$$A(n) := \sum_{k \geq 0} \binom{n}{k}^2 \binom{n+k}{k}^2.$$

These numbers arose in Apéry's proof of the irrationality of  $\zeta(3)$ . This sum is finite, since  $\binom{n}{k} = 0$  when  $k > n$ . The sequence  $A(n)_{n \geq 0}$  is

$$1, 5, 73, 1445, 33001, 819005, 21460825, 584307365, \dots$$

The Apéry numbers satisfy the recurrence

$$(1) \quad n^3 A(n) - (34n^3 - 51n^2 + 27n - 5)A(n-1) + (n-1)^3 A(n-2) = 0$$

for all integers  $n \geq 2$ .

Exceptional properties of the Apéry sequence have been observed in many settings [14]. Gessel [5] showed that the Apéry numbers satisfy the Lucas congruence

$$(2) \quad A(d+pn) \equiv A(d)A(n) \pmod{p}$$

for all  $d \in \{0, 1, \dots, p-1\}$  and  $n \geq 0$ . Beukers [1] established the supercongruence  $A(p^\alpha n - 1) \equiv A(p^{\alpha-1}n - 1) \pmod{p^{3\alpha}}$  for all primes  $p \geq 5$ , and Straub [11] showed that a related supercongruence holds more generally for a four-dimensional sequence containing  $A(n)_{n \geq 0}$  as its diagonal.

Gessel also extended Congruence (2) to a congruence modulo  $p^2$  as follows. Define the sequence  $A'(n)_{n \geq 0}$  by

$$(3) \quad A'(n) := 2 \sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{k}^2 (H_{n+k} - H_{n-k}),$$

where  $H_k = 1 + \frac{1}{2} + \dots + \frac{1}{k}$  is the  $k$ th harmonic number. The sequence  $A'(n)_{n \geq 0}$  is

$$0, 12, 210, 4438, 104825, \frac{13276637}{5}, 70543291, \frac{67890874657}{35}, \dots$$

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<sup>1</sup>This paper was originally posted on the arXiv by the first two authors. Christian Krattenthaler became a coauthor after improving the proof of Theorem 1.

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Then

$$(4) \quad A(d + pn) \equiv (A(d) + pnA'(d))A(n) \pmod{p^2}$$

for all  $d \in \{0, 1, \dots, p-1\}$  and for all  $n \geq 0$  [5, Theorem 4].

Gessel remarks that if  $A(n)$  can be extended to a differentiable function  $A(x)$  defined for  $x \in \mathbb{R}_{\geq 0}$  such that  $A(x)$  satisfies Recurrence (1), then  $A'(n) = \left(\frac{d}{dx}A(x)\right)|_{x=n}$ . As shown by Zagier [14, Proposition 1] and proved in an automated way by Osburn and Straub [9, Remark 2.5],  $A(n)$  can be extended to an entire function  $A(z)$  satisfying

$$(5) \quad \begin{aligned} z^3A(z) - (34z^3 - 51z^2 + 27z - 5)A(z-1) + (z-1)^3A(z-2) \\ = \frac{8}{\pi^2}(2z-1)(\sin(\pi z))^2 \end{aligned}$$

for all  $z \in \mathbb{C}$ . Since both  $\frac{8}{\pi^2}(2z-1)(\sin(\pi z))^2$  and its derivative vanish at integer values of  $z$ , it follows that  $A'(n) = \left(\frac{d}{dz}A(z)\right)|_{z=n}$ , hence the notation  $A'(n)$ . Therefore the extension  $A(z)$  confirms Gessel's intuition.

In this article we write the coefficients in the Taylor series of  $A(z) = \sum_{m \geq 0} a_m z^m$  at  $z = 0$  as an explicit  $\mathbb{Z}$ -linear combination of multiple zeta values. A striking fact is that the coefficient of each multiple zeta value is a signed power of 2. Let  $s_1, s_2, \dots, s_j$  be positive integers with  $s_1 \geq 2$ . The *multiple zeta value*  $\zeta(s_1, s_2, \dots, s_j)$  is defined as

$$\zeta(s_1, s_2, \dots, s_j) := \sum_{n_1 > n_2 > \dots > n_j > 0} \frac{1}{n_1^{s_1} n_2^{s_2} \dots n_j^{s_j}}.$$

The *weight* of  $\zeta(s_1, s_2, \dots, s_j)$  is  $s_1 + s_2 + \dots + s_j$ .

Let  $\chi(m)$  be the characteristic function of the set of odd numbers. That is,  $\chi(m) = 0$  if  $m$  is even and  $\chi(m) = 1$  if  $m$  is odd. For a tuple  $\mathbf{s} = (s_1, s_2, \dots, s_j)$ , let  $e(\mathbf{s}) = |\{i : 2 \leq i \leq j \text{ and } s_i = 2\}|$ .

**Theorem 1.** *Let  $A(z) = \sum_{m \geq 0} a_m z^m$  be the Apéry function. For each  $m \geq 1$ ,*

$$a_m = \sum_{\mathbf{s}} (-1)^{\frac{m-s_1}{2}} 2^{e(\mathbf{s})+\chi(m)} \zeta(s_1, s_2, \dots, s_j),$$

where the sum is over all tuples  $\mathbf{s} = (s_1, s_2, \dots, s_j)$ , with  $j \geq 1$ , of non-negative integers satisfying

- $s_1 + s_2 + \dots + s_j = m$ ,
- $s_1 = 3$  if  $m$  is odd and  $s_1 \in \{2, 4\}$  if  $m$  is even, and
- $s_i \in \{2, 4\}$  for all  $i \in \{2, \dots, j\}$ .

The first several coefficients are

$$\begin{aligned}
a_0 &= 1 \\
a_1 &= 0 \\
a_2 &= \zeta(2) \\
a_3 &= 2\zeta(3) \\
a_4 &= \zeta(4) - 2\zeta(2, 2) \\
a_5 &= -4\zeta(3, 2) \\
a_6 &= \zeta(2, 4) - 2\zeta(4, 2) + 4\zeta(2, 2, 2) \\
a_7 &= 2\zeta(3, 4) + 8\zeta(3, 2, 2) \\
a_8 &= \zeta(4, 4) - 2\zeta(2, 2, 4) - 2\zeta(2, 4, 2) + 4\zeta(4, 2, 2) - 8\zeta(2, 2, 2, 2) \\
a_9 &= -4\zeta(3, 2, 4) - 4\zeta(3, 4, 2) - 16\zeta(3, 2, 2, 2).
\end{aligned}$$

Let  $F(m)$  be the  $m$ th Fibonacci number. Since the number of integer compositions of  $m$  using parts 1 and 2 is  $F(m+1)$ , Theorem 1 expresses  $a_m$  as a linear combination of  $F(\frac{m}{2} + 1)$  multiple zeta values if  $m$  is even and  $F(\frac{m-1}{2})$  multiple zeta values if  $m$  is odd.

Let  $P(m)$  be the number of integer compositions of  $m - 3$  using parts 2 and 3. Then  $P(m)$  is the  $m$ th Padovan number and satisfies the recurrence  $P(m) = P(m-2) + P(m-3)$  with initial conditions  $P(3) = 1$ ,  $P(4) = 0$ ,  $P(5) = 1$ . Let  $d_m$  be the dimension of the  $\mathbb{Q}$ -vector space spanned by the weight- $m$  multiple zeta values. Recent progress by Brown [2] and Zagier [13] shows that  $d_m \leq P(m+3)$ . For  $m \geq 13$ , the representation of  $a_m$  in Theorem 1 uses fewer than  $P(m+3)$  multiple zeta values. Since  $F(\frac{m}{2} + 1) > P(m+3)$  for  $m \in \{4, 6, 8, 10, 12\}$ , this implies that  $a_4, a_6, a_8, a_{10}, a_{12}$  can be written as  $\mathbb{Q}$ -linear combinations of fewer multiple zeta values than Theorem 1 provides. Namely,

$$\begin{aligned}
a_4 &= -\frac{1}{2}\zeta(4) \\
a_6 &= \frac{3}{2}\zeta(6) - 3\zeta(4, 2) \\
a_8 &= -\frac{13}{24}\zeta(8) + 6\zeta(4, 2, 2) \\
a_{10} &= \frac{7}{8}\zeta(10) + 3\zeta(2, 4, 4) - 12\zeta(4, 2, 2, 2) \\
a_{12} &= -\frac{915}{22112}\zeta(12) + 6\zeta(4, 2, 2, 4) + 6\zeta(4, 2, 4, 2) + 6\zeta(4, 4, 2, 2) + 24\zeta(4, 2, 2, 2, 2).
\end{aligned}$$

We prove Theorem 1 in Section 2. The proof technique can also be applied to compute the Taylor coefficients for a larger family of hypergeometric functions. We remark that there are some parallels between Theorem 1 and work of Cresson, Fischler, and Rivoal [3], who show that a class of hypergeometric series can be decomposed as  $\mathbb{Q}$ -linear combinations of multiple zeta values.

Returning to congruences for  $A(n)$  in Section 3, we consider the following question. For which base- $p$  digits  $d$  does Congruence (2) hold not just modulo  $p$  but modulo  $p^2$ ? The following theorem characterizes such digits. Let

$$D(p) = \{d \in \{0, 1, \dots, p-1\} : A(d) \equiv A(p-1-d) \pmod{p^2}\}.$$

**Theorem 2.** *Let  $p$  be a prime, and let  $d \in \{0, 1, \dots, p-1\}$ . The congruence  $A(d+pn) \equiv A(d)A(n) \pmod{p^2}$  holds for all  $n \in \mathbb{Z}$  if and only if  $d \in D(p)$ .*

In particular, if  $n$  is a non-negative integer and all digits in its standard base- $p$  representation  $n_\ell \cdots n_1 n_0$  belong to  $D(p)$ , then

$$A(n) \equiv A(n_0)A(n_1) \cdots A(n_\ell) \pmod{p^2}.$$

## 2. TAYLOR COEFFICIENTS OF THE APÉRY FUNCTION

In this section we give a proof of Theorem 1. Let  $\mathbb{N} = \{0, 1, 2, \dots\}$ . The sequence  $A(n)_{n \geq 0}$  can be interpolated to  $\mathbb{C}$  using the gamma function  $\Gamma(z)$ . Recall that  $\Gamma(z)$  is a meromorphic function satisfying

$$\Gamma(1) = 1 \text{ and } \Gamma(z+1) = z\Gamma(z)$$

for  $z \notin -\mathbb{N}$ . The gamma function has simple poles at the non-positive integers.

For  $n \geq 0$ , we can write  $A(n)$  as

$$\begin{aligned} A(n) &= \sum_{k \geq 0} \binom{n}{k}^2 \binom{n+k}{k}^2 \\ &= \sum_{k \geq 0} \frac{\Gamma(n+k+1)^2}{\Gamma(n-k+1)^2 \Gamma(k+1)^4}. \end{aligned}$$

We extend  $A(n)$  to complex values by defining

$$A(z) = \sum_{k \geq 0} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2 \Gamma(k+1)^4}.$$

Note that for each  $k \in \mathbb{N}$ , the function  $\frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2 \Gamma(k+1)^4}$  is a polynomial in  $z$ . Furthermore for each  $z \in \mathbb{C}$ , the series  $\sum_{k \geq 0} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2 \Gamma(k+1)^4}$  is locally uniformly convergent. Thus  $A(z)$  is an entire function, which we call the *Apéry function*. We remark that  $A(z)$  can be written using the hypergeometric function  ${}_4F_3$ . Let  $(z)_k := z(z+1)(z+2) \cdots (z+k-1)$  be the Pochhammer symbol (rising factorial). By writing  $\frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2} = (-z)_k^2 (z+1)_k^2$ , we see that

$$\begin{aligned} (6) \quad A(z) &= \sum_{k \geq 0} \frac{(-z)_k^2 (z+1)_k^2}{k!^4} \\ &= {}_4F_3(-z, -z, z+1, z+1; 1, 1, 1; 1). \end{aligned}$$

Straub [11, Remark 1.3] proved the reflection formula  $A(-1-n) = A(n)$  for all  $n \in \mathbb{Z}$ . Equation (6) shows that this formula also holds for non-integers, since the hypergeometric series is invariant under replacing  $z$  with  $-1-z$ .

**Proposition 3.** *For all  $z \in \mathbb{C}$ , we have  $A(-1-z) = A(z)$ .*

Figure 1 shows this symmetry on the real line. In light of Proposition 3, Theorem 1 also gives us the Taylor expansion of  $A(z)$  at  $z = -1$  for free. We note that at the symmetry point  $x = -\frac{1}{2}$ , Zagier has shown that  $A(-\frac{1}{2}) = \frac{16}{\pi^2} L(f, 2)$  where  $L(f, 2)$  is the critical  $L$ -value of  $f$ , the unique normalized Hecke eigenform of weight 4 for  $\Gamma_0(8)$ ; see [14] for an account and [15] for a generalization. There is no reason to expect that the Taylor coefficients of  $A(z)$  centered at non-integer points are  $\mathbb{Q}$ -linear combinations of multiple zeta values.

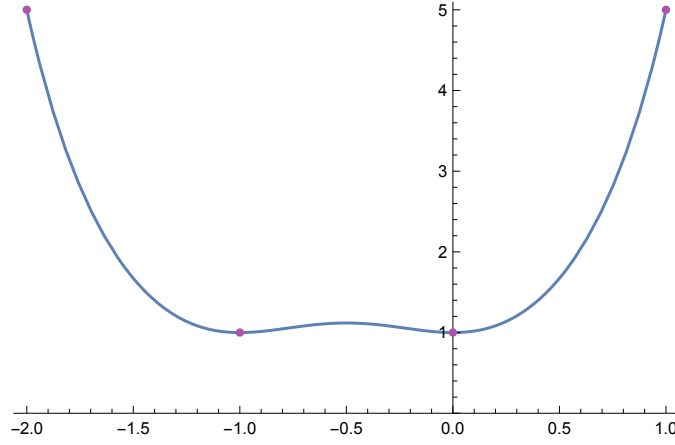


FIGURE 1. A plot of  $A(z)$  for real  $z$  in the interval  $-2 \leq z \leq 1$ , showing the reflection symmetry  $A(-1-z) = A(z)$ .

Let

$$(7) \quad A(z) = \sum_{k \geq 0} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2 \Gamma(k+1)^4} = \sum_{m \geq 0} a_m z^m$$

be the Taylor series expansion of the Apéry function centered at the origin. It is possible to compute  $a_m$  by directly evaluating the  $m$ th derivative  $A^{(m)}(z)$  at  $z = 0$ .

**Example 4.** The derivative of the summand is

$$\frac{1}{k!^4} \frac{d}{dz} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2} = \frac{1}{k!^4} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2} (2\psi(z+k+1) - 2\psi(z-k+1)),$$

where the digamma function  $\psi(z) := \frac{\Gamma'(z)}{\Gamma(z)}$  is the logarithmic derivative of  $\Gamma(z)$ .

This agrees with the expression for  $A'(n)$  in Equation (3). Since  $\frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2} = O(z^2)$  as  $z \rightarrow 0$  and  $2\psi(z+k+1) - 2\psi(z-k+1)$  has a simple pole at 0 for each  $k$ , we have  $a_1 = \frac{A'(0)}{1!} = 0$ . Similarly, the second derivative is

$$\begin{aligned} \frac{1}{k!^4} \frac{d^2}{dz^2} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2} &= \frac{1}{k!^4} \frac{\Gamma(z+k+1)^2}{\Gamma(z-k+1)^2} (4\psi(z+k+1)^2 + 2\psi'(z+k+1) \\ &\quad - 8\psi(z+k+1)\psi(z-k+1) + 4\psi(z-k+1)^2 - 2\psi'(z-k+1)). \end{aligned}$$

The series expansions of  $\psi(z+k+1)$  and  $\psi(z-k+1)$  imply  $A''(0) = \sum_{k \geq 1} \frac{2}{k^2} = 2\zeta(2)$ , so  $a_2 = \frac{A''(0)}{2!} = \zeta(2)$ .

Theorem 1 can be proved by carrying out the same approach for general  $m$ . However, we give a shorter proof in the spirit of [4, Section 1.4].

*Proof of Theorem 1.* We consider the summand in Equation (7). For  $k = 0$ , we have  $\frac{\Gamma^2(z+k+1)}{\Gamma^2(z-k+1)k!^4} = 1$ . For  $k \geq 1$ , we have

$$\begin{aligned}
 \frac{\Gamma^2(z+k+1)}{\Gamma^2(z-k+1)k!^4} &= \frac{(z-k+1)^2 \cdots (z-1)^2 z^2 (z+1)^2 \cdots (z+k)^2}{k!^4} \\
 &= \left(1 - \frac{z}{k-1}\right)^2 \cdots \left(1 - \frac{z}{1}\right)^2 \left(1 + \frac{z}{1}\right)^2 \cdots \left(1 + \frac{z}{k-1}\right)^2 \frac{z^2}{k^2} \left(1 + \frac{z}{k}\right)^2 \\
 &= \left(1 - \frac{z^2}{(k-1)^2}\right)^2 \cdots \left(1 - \frac{z^2}{1^2}\right)^2 \frac{z^2}{k^2} \left(1 + \frac{z}{k}\right)^2 \\
 (8) \quad &= \left(1 - 2\frac{z^2}{1^2} + \frac{z^4}{1^4}\right) \cdots \left(1 - 2\frac{z^2}{(k-1)^2} + \frac{z^4}{(k-1)^4}\right) \left(\frac{z^2}{k^2} + 2\frac{z^3}{k^3} + \frac{z^4}{k^4}\right).
 \end{aligned}$$

Recall that  $\chi(m)$  is the characteristic function of the set of odd numbers, and  $e(\mathbf{s}) = |\{i : 2 \leq i \leq j \text{ and } s_i = 2\}|$  for a tuple  $\mathbf{s} = (s_1, s_2, \dots, s_j)$ . By expanding the product (8) to extract the coefficient of  $z^m$ , one sees that this coefficient equals

$$\sum_{\substack{\mathbf{s}=(s_1,\dots,s_j) \\ s_1+\dots+s_j=m}} \sum_{k=n_1>n_2>\dots>n_j>0} (-1)^{\frac{m-s_1}{2}} 2^{e(\mathbf{s})+\chi(m)} \frac{1}{n_1^{s_1} n_2^{s_2} \cdots n_j^{s_j}},$$

where the outer sum is over all  $\mathbf{s}$  described in the statement of Theorem 1. Now we sum over all  $k$  to obtain  $a_m$ , and the statement follows.  $\square$

As discussed in Section 1, the coefficients  $a_4, a_6, a_8, a_{10}, a_{12}$  can be written as  $\mathbb{Q}$ -linear combinations of fewer multiple zeta values than given by Theorem 1. The strategy given in the following example can be used to reduce  $a_m$  for all even  $m \geq 4$ .

**Example 5.** For  $m = 10$ , Theorem 1 gives

$$\begin{aligned}
 a_{10} &= \zeta(2, 4, 4) - 2\zeta(4, 2, 4) - 2\zeta(4, 4, 2) \\
 &\quad + 4\zeta(2, 2, 2, 4) + 4\zeta(2, 2, 4, 2) + 4\zeta(2, 4, 2, 2) - 8\zeta(4, 2, 2, 2) \\
 &\quad + 16\zeta(2, 2, 2, 2, 2).
 \end{aligned}$$

We will rewrite several products  $\zeta(s_1, s_2, \dots, s_j)\zeta(i)$  as linear combinations of multiple zeta values. For example,

$$\begin{aligned}
 &\left(\sum_{k_1>k_2>0} \frac{1}{k_1^a k_2^b}\right) \left(\sum_{k_3>0} \frac{1}{k_3^c}\right) \\
 &= \sum_{k_3>k_1>k_2>0} \frac{1}{k_1^a k_2^b k_3^c} + \sum_{k_1>k_3>k_2>0} \frac{1}{k_1^a k_2^b k_3^c} + \sum_{k_1>k_2>k_3>0} \frac{1}{k_1^a k_2^b k_3^c} \\
 &\quad + \sum_{k_1>k_2>0} \frac{1}{k_1^{a+c} k_2^b} + \sum_{k_1>k_2>0} \frac{1}{k_1^a k_2^{b+c}},
 \end{aligned}$$

so that

$$(9) \quad \zeta(a, b)\zeta(c) = \zeta(c, a, b) + \zeta(a, c, b) + \zeta(a, b, c) + \zeta(a+c, b) + \zeta(a, b+c).$$

As in the derivation of Equation (9), we have  $\zeta(a)\zeta(b) = \zeta(a, b) + \zeta(b, a) + \zeta(a+b)$ .

We first express  $-2\zeta(4, 2, 4) - 2\zeta(4, 4, 2)$  in terms of  $\zeta(2, 4, 4)$  and  $\zeta(10)$ . By (9) we have

$$\zeta(4, 4)\zeta(2) = \zeta(2, 4, 4) + \zeta(4, 2, 4) + \zeta(4, 4, 2) + \zeta(6, 4) + \zeta(4, 6).$$

The relations  $\zeta(4)\zeta(4) = 2\zeta(4, 4) + \zeta(8)$  and  $\zeta(4)\zeta(6) = \zeta(4, 6) + \zeta(6, 4) + \zeta(10)$  allow us to write

$$\begin{aligned} -2\zeta(4, 2, 4) - 2\zeta(4, 4, 2) &= 2\zeta(2, 4, 4) + 2\zeta(4)\zeta(6) - 2\zeta(10) - \zeta(4)^2\zeta(2) + \zeta(8)\zeta(2) \\ &= 2\zeta(2, 4, 4) - \frac{3}{40}\zeta(10) \end{aligned}$$

using  $\zeta(2) = \frac{\pi^2}{6}$ ,  $\zeta(4) = \frac{\pi^4}{90}$ ,  $\zeta(6) = \frac{\pi^6}{945}$ ,  $\zeta(8) = \frac{\pi^8}{9450}$ , and  $\zeta(10) = \frac{\pi^{10}}{93555}$ . Next we rewrite

$$4\zeta(2, 2, 2, 4) + 4\zeta(2, 2, 4, 2) + 4\zeta(2, 4, 2, 2).$$

For this we use

$$\begin{aligned} \zeta(2, 2, 2)\zeta(4) - \zeta(2, 2, 2, 4) - \zeta(2, 2, 4, 2) - \zeta(2, 4, 2, 2) - \zeta(4, 2, 2, 2) \\ = \zeta(2, 2, 6) + \zeta(2, 6, 2) + \zeta(6, 2, 2) \\ = \zeta(2, 2)\zeta(6) - (\zeta(8, 2) + \zeta(2, 8)) \\ = \zeta(2, 2)\zeta(6) - (\zeta(2)\zeta(8) - \zeta(10)). \end{aligned}$$

Therefore  $4\zeta(2, 2, 2, 4) + 4\zeta(2, 2, 4, 2) + 4\zeta(2, 4, 2, 2)$  can be written using  $\zeta(2, 2)\zeta(6)$ ,  $\zeta(2, 2, 2)\zeta(4)$ ,  $\zeta(4, 2, 2, 2)$ , and  $\zeta(10)$ . Finally, we use

$$\zeta(\underbrace{2, \dots, 2}_j) = \frac{\pi^{2j}}{(2j+1)!}$$

(see for example [7]) to write  $\zeta(2, 2)$ ,  $\zeta(2, 2, 2)$ , and  $\zeta(2, 2, 2, 2, 2)$ . Consolidating these results, we obtain

$$a_{10} = \frac{7}{8}\zeta(10) + 3\zeta(2, 4, 4) - 12\zeta(4, 2, 2, 2).$$

### 3. LUCAS CONGRUENCES MODULO $p^2$

Gessel [5] proved three theorems on congruences for  $A(n)$  where  $n \geq 0$ . In this section we generalize these theorems to  $n \in \mathbb{Z}$ , making substantial use of the reflection formula  $A(-1-z) = A(z)$  from Proposition 3. We simplify one of the arguments by using the fact that we can differentiate  $A(z)$ . We then use these congruences to prove Theorem 2.

First we generalize Gessel's result that the Apéry numbers satisfy a Lucas congruence modulo  $p$  [5, Theorem 1].

**Theorem 6.** *Let  $p$  be a prime. For all  $d \in \{0, 1, \dots, p-1\}$  and for all  $n \in \mathbb{Z}$ , we have  $A(d+pn) \equiv A(d)A(n) \pmod{p}$ .*

*Proof.* Gessel proved the statement for  $n \geq 0$ . Let  $n \leq -1$ . By Proposition 3,

$$\begin{aligned} A(d+pn) &= A(-1-(d+pn)) \\ &= A((p-1-d)+p(-1-n)) \\ &\equiv A(p-1-d)A(-1-n) \pmod{p} \\ &= A(p-1-d)A(n). \end{aligned}$$

Malik and Straub [8, Lemma 6.2] proved that  $A(p-1-d) \equiv A(d) \pmod{p}$ , which completes the proof.  $\square$

Next we generalize Gessel's congruence for  $A(pn)$  modulo  $p^3$  for  $p \geq 5$  and variants for  $p = 2$  and  $p = 3$  [5, Theorem 3].

**Theorem 7.** *For all  $n \in \mathbb{Z}$ ,*

- $A(n) \equiv 5^n \pmod{8}$  for all  $n \geq 0$  and  $A(n) \equiv 5^{n+1} \pmod{8}$  for all  $n \leq -1$ ,
- $A(d+3n) \equiv A(d)A(n) \pmod{9}$  for all  $d \in \{0, 1, 2\}$ , and
- $A(pn) \equiv A(n) \equiv A(pn+p-1) \pmod{p^3}$  for all primes  $p \geq 5$ .

A special case of a theorem of Straub [11, Theorem 1.2] shows that  $A(pn) \equiv A(n) \pmod{p^3}$  for all  $n \in \mathbb{Z}$  and all primes  $p \geq 5$ . We prove this result another way, using an approach similar to Gessel's.

*Proof of Theorem 7.* Gessel proved  $A(n) \equiv 5^n \pmod{8}$  for all  $n \geq 0$ . For  $n \leq -1$ , we use Proposition 3 to write

$$\begin{aligned} A(n) &= A(-1-n) \equiv 5^{-1-n} \pmod{8} \\ &\equiv 5^{1+n} \pmod{8} \end{aligned}$$

since  $5^{-1} \equiv 5 \pmod{8}$ .

For  $p = 3$ , the proof is similar to the proof of Theorem 6. Gessel proved the statement for  $n \geq 0$ , so for  $n \leq -1$  we have

$$\begin{aligned} A(d+3n) &= A(-1-(d+3n)) \\ &= A((2-d)+3(-1-n)) \\ &\equiv A(2-d)A(-1-n) \pmod{9} \\ &\equiv A(d)A(n) \pmod{9} \end{aligned}$$

since one checks that  $A(2-d) \equiv A(d) \pmod{9}$ .

Let  $p \geq 5$ . Gessel proved  $A(pn) \equiv A(n) \pmod{p^3}$  for all  $n \geq 0$ . We show  $A(pn+p-1) \equiv A(n) \pmod{p^3}$  for all  $n \geq 0$ . We write

$$\begin{aligned} A(pn+p-1) &= \sum_{k=0}^{pn+p-1} \binom{pn+p-1}{k}^2 \binom{pn+p-1+k}{k}^2 \\ &= \sum_{d=0}^{p-1} \sum_{m=0}^n \binom{pn+p-1}{pm+d}^2 \binom{p(n+m+1)+d-1}{pm+d}^2 \\ &= \sum_{d=0}^{p-1} \sum_{m=0}^n \binom{pn+p-1}{pm+d}^2 \frac{p^2(n+1)^2}{(p(n+m+1)+d)^2} \binom{p(n+m+1)+d}{pm+d}^2 \\ &= S_0 + S_1 \end{aligned}$$

where

$$S_0 = \sum_{m=0}^n \binom{pn+p-1}{pm}^2 \frac{(n+1)^2}{(n+m+1)^2} \binom{p(n+m+1)}{pm}^2$$

is the summand for  $d = 0$ , and

$$S_1 = \sum_{d=1}^{p-1} \sum_{m=0}^n \binom{pn+p-1}{pm+d}^2 \frac{p^2(n+1)^2}{(p(n+m+1)+d)^2} \binom{p(n+m+1)+d}{pm+d}^2.$$



For  $S_0$ , we have

$$\begin{aligned}
S_0 &= \sum_{m=0}^n \frac{(pn + p - pm)^2}{(pn + p)^2} \binom{pn + p}{pm}^2 \frac{(n+1)^2}{(n+m+1)^2} \binom{p(n+m+1)}{pm}^2 \\
&\equiv \sum_{m=0}^n \frac{(n-m+1)^2}{(n+m+1)^2} \binom{n+1}{m}^2 \binom{n+m+1}{m}^2 \pmod{p^3} \\
&= \sum_{m=0}^n \binom{n}{m}^2 \binom{n+m}{m}^2 \\
&= A(n)
\end{aligned}$$

by Ljunggren's congruence  $\binom{pa}{pb} \equiv \binom{a}{b} \pmod{p^3}$ , which holds for all primes  $p \geq 5$  [6].

For  $S_1$ , we have

$$\begin{aligned}
S_1 &\equiv p^2 \sum_{d=1}^{p-1} \sum_{m=0}^n \binom{pn + p - 1}{pm + d}^2 \frac{(n+1)^2}{d^2} \binom{p(n+m+1) + d}{pm + d}^2 \pmod{p^3} \\
&\equiv p^2 \sum_{d=1}^{p-1} \sum_{m=0}^n \binom{p-1}{d}^2 \binom{n}{m}^2 \frac{(n+1)^2}{d^2} \binom{d}{d}^2 \binom{n+m+1}{m}^2 \pmod{p^3}
\end{aligned}$$

by the Lucas congruence for binomial coefficients modulo  $p$ . Since

$$\binom{p-1}{d} = \frac{(p-1)(p-2)\cdots(p-d)}{1 \cdot 2 \cdots d} \equiv \frac{(-1)(-2)\cdots(-d)}{1 \cdot 2 \cdots d} \equiv (-1)^d \pmod{p},$$

we obtain

$$\begin{aligned}
S_1 &\equiv p^2 \left( \sum_{d=1}^{p-1} \frac{1}{d^2} \right) \sum_{m=0}^n \binom{n}{m}^2 (n+1)^2 \binom{n+m+1}{m}^2 \pmod{p^3} \\
&\equiv 0 \pmod{p^3}
\end{aligned}$$

since  $\sum_{d=1}^{p-1} \frac{1}{d^2} \equiv 0 \pmod{p}$ , as established by Wolstenholme [12]. Therefore  $A(pn + p - 1) = S_0 + S_1 \equiv A(n) \pmod{p^3}$ .

Now for  $n \leq -1$  we have

$$\begin{aligned}
A(pn) &= A(-1 - pn) \\
&= A((p-1) + p(-1-n)) \\
&\equiv A(-1-n) \pmod{p^3} \\
&= A(n)
\end{aligned}$$

and

$$\begin{aligned}
A(pn + p - 1) &= A(-1 - (pn + p - 1)) \\
&= A(p(-1-n)) \\
&\equiv A(-1-n) \pmod{p^3} \\
&= A(n).
\end{aligned}$$

□

Finally, we generalize Gessel's congruence for  $A(d+pn)$  modulo  $p^2$  [5, Theorem 4]. Recall that  $A'(n)$  is given by Equation (3). Since  $A'(n) \in \mathbb{Q}$  for every  $n \geq 0$ , it follows that if the denominator of  $A'(n)$  is not divisible by  $p$  then we can interpret  $A'(n)$  modulo  $p^2$ .

**Theorem 8.** *Let  $p$  be a prime, and let  $d \in \{0, 1, \dots, p-1\}$ . The denominator of  $A'(d)$  is not divisible by  $p$ . Moreover, for all  $n \in \mathbb{Z}$ ,*

$$(10) \quad A(d+pn) \equiv (A(d) + pnA'(d))A(n) \pmod{p^2}$$

*Proof.* Gessel proved the statement for  $n \geq 0$ . The same approach allows us to prove the general case.

Fix  $n \in \mathbb{Z}$ . For each  $d \in \{0, 1, \dots, p-1\}$ , define  $c_d \in \{0, 1, \dots, p-1\}$  such that  $A(d+pn) \equiv A(d)A(n) + pc_d \pmod{p^2}$ ; this can be done by Theorem 6. Let  $c_{-1} = 0$ . (The value of  $c_{-1}$  does not actually matter, since it will be multiplied by 0.) We show that  $(c_d)_{0 \leq d \leq p-1}$  and  $(nA'(d)A(n))_{0 \leq d \leq p-1}$  satisfy the same recurrence and initial conditions modulo  $p$ ; this will imply  $c_d \equiv nA'(d)A(n) \pmod{p}$ . Theorem 7 implies that  $A(pn) \equiv A(n) \pmod{p^2}$ , so  $c_0 = 0$ . Since  $A'(0) = 0$ , the initial conditions are equal.

Let  $d \in \{1, 2, \dots, p-1\}$ . Write Equation (1) as

$$(11) \quad \sum_{i=0}^2 r_i(n)A(n-i) = 0,$$

where each  $r_i(n)$  is a polynomial in  $n$  with integer coefficients. Note that Equation (11) holds for all  $n \in \mathbb{Z}$ . Substituting  $d+pn$  for  $n$  in Equation (11) gives

$$\sum_{i=0}^2 r_i(d+pn)A(d-i+pn) = 0.$$

If  $d-i = -1$  then  $r_i(d+pn) = r_2(1+pn) = (pn)^3 \equiv 0 \pmod{p^2}$ , hence the arbitrary value of  $c_{-1}$ . Therefore, using the Taylor expansion of  $r_i(n)$ , we have

$$\sum_{i=0}^2 (r_i(d) + pnr'_i(d))(A(d-i)A(n) + pc_{d-i}) \equiv 0 \pmod{p^2}.$$

Since  $\sum_{i=0}^2 r_i(d)A(d-i) = 0$ , expanding and dividing by  $p$  gives

$$\sum_{i=0}^2 (r_i(d)c_{d-i} + nr'_i(d)A(d-i)A(n)) \equiv 0 \pmod{p}.$$

This gives a recurrence satisfied by  $(c_d)_{0 \leq d \leq p-1}$  that can be used to compute  $c_1, c_2, \dots, c_{p-1}$  since  $r_0(d) = d^3 \not\equiv 0 \pmod{p}$ .

To obtain a recurrence for  $(nA'(d)A(n))_{0 \leq d \leq p-1}$ , we differentiate Equation (5) to obtain

$$\sum_{i=0}^2 (r_i(d)A'(d-i) + r'_i(d)A(d-i)) = 0.$$

Since  $A'(0)$  and  $A'(1)$  are integers and  $r_0(d) \not\equiv 0 \pmod{p}$ , the denominator of  $A'(d)$  is not divisible by  $p$ . By multiplying by  $nA(n)$ , we obtain

$$\sum_{i=0}^2 (r_i(d)nA'(d-i)A(n) + nr'_i(d)A(d-i)A(n)) = 0.$$

By subtracting this from the recurrence for  $(c_d)_{0 \leq d \leq p-1}$ , we see that

$$\sum_{i=0}^2 r_i(d)(c_{d-i} - nA'(d-i)A(n)) \equiv 0 \pmod{p}.$$

Since  $r_0(d) \not\equiv 0 \pmod{p}$ , it follows that  $c_d \equiv nA'(d)A(n) \pmod{p}$  for all  $d \in \{0, 1, \dots, p-1\}$ .  $\square$

In the case  $p = 3$ , Theorem 8 gives a second proof of the congruence  $A(d+3n) \equiv A(d)A(n) \pmod{9}$  from Theorem 7, since  $A'(0) \equiv A'(1) \equiv A'(2) \equiv 0 \pmod{3}$ . For larger primes, in general  $A(d+pn) \not\equiv A(d)A(n) \pmod{p^2}$ . However, if we restrict to certain sets of base- $p$  digits, then we do obtain congruences that hold modulo  $p^2$ . For example, if  $d \in \{0, 2, 4\}$ , then

$$A(d+5n) \equiv A(d)A(n) \pmod{25}.$$

This was proven by the authors [10] by computing an automaton for  $A(n) \pmod{25}$ . Since  $A(0) \equiv 1 \equiv A(4) \pmod{25}$  and  $A(2) \equiv 23 \pmod{25}$ , this implies  $A(n) \equiv 23^{e_2(n)} \pmod{25}$  for all  $n \geq 0$  whose base-5 digits belong to  $\{0, 2, 4\}$ , where  $e_2(n)$  is the number of 2s in the base-5 representation of  $n$ . The following theorem generalizes this result to other primes.

We say that the set  $D \subseteq \{0, 1, \dots, p-1\}$  supports a *Lucas congruence* for the sequence  $s(n)_{n \in \mathbb{Z}}$  modulo  $p^\alpha$  if  $s(d+pn) \equiv s(d)s(n) \pmod{p^\alpha}$  for all  $d \in D$  and for all  $n \in \mathbb{Z}$ . As mentioned in the proof of Theorem 6, Malik and Straub [8, Lemma 6.2] proved that  $A(d) \equiv A(p-1-d) \pmod{p}$  for each  $d \in \{0, 1, \dots, p-1\}$ . Let  $D(p)$  be the set of base- $p$  digits for which this congruence holds modulo  $p^2$ ; that is,

$$D(p) = \{d \in \{0, 1, \dots, p-1\} : A(d) \equiv A(p-1-d) \pmod{p^2}\}.$$

**Theorem 9.** *The set  $D(p)$  is the maximum set of digits that supports a Lucas congruence for the Apéry numbers modulo  $p^2$ .*

*Proof.* Let  $d \in D(p)$ , so that  $A(d) \equiv A(p-1-d) \pmod{p^2}$ . Letting  $n = -1$  in Theorem 8 gives  $A(d-p) \equiv A(d) - pA'(d) \pmod{p^2}$ . Applying Proposition 3, we find

$$\begin{aligned} pA'(d) &\equiv A(d) - A(d-p) \pmod{p^2} \\ &= A(d) - A(p-1-d) \\ &\equiv 0 \pmod{p^2}. \end{aligned}$$

Therefore it follows from Theorem 8 that, for all  $n \in \mathbb{Z}$ ,

$$\begin{aligned} A(d+pn) &\equiv (A(d) + pnA'(d))A(n) \pmod{p^2} \\ &\equiv A(d)A(n) \pmod{p^2}. \end{aligned}$$

Therefore  $D(p)$  supports a Lucas congruence for the Apéry numbers modulo  $p^2$ .

To see that  $D(p)$  is the maximum such set, assume  $A(d+pn) \equiv A(d)A(n) \pmod{p^2}$  for all  $n \in \mathbb{Z}$ . Then

$$\begin{aligned} (A(d) + pnA'(d))A(n) &\equiv A(d+pn) \pmod{p^2} \\ &\equiv A(d)A(n) \pmod{p^2}, \end{aligned}$$

and it follows that  $pnA'(d)A(n) \equiv 0 \pmod{p^2}$  for all  $n \in \mathbb{Z}$ . Therefore  $A(d) - A(p-1-d) = A(d) - A(d-p) \equiv pA'(d) \equiv 0 \pmod{p^2}$ .  $\square$

As a special case, we obtain the following congruence, since  $\{0, p-1\} \subseteq D(p)$  by Theorem 7, and  $A(0) = 1 \equiv A(p-1) \pmod{p^2}$ .

**Corollary 10.** *Let  $p \neq 2$  and  $n \geq 0$ . If the base- $p$  digits of  $n$  all belong to  $\{0, \frac{p-1}{2}, p-1\}$ , then  $A(n) \equiv A(\frac{p-1}{2})^{e(n)} \pmod{p^2}$  where  $e(n)$  is the number of occurrences of the digit  $\frac{p-1}{2}$ .*

These are the first several primes with digit sets  $D(p)$  containing at least 4 digits:

$p$	$D(p)$
7	$\{0, 2, 3, 4, 6\}$
23	$\{0, 7, 11, 15, 22\}$
43	$\{0, 5, 18, 21, 24, 37, 42\}$
59	$\{0, 6, 29, 52, 58\}$
79	$\{0, 18, 39, 60, 78\}$
103	$\{0, 17, 51, 85, 102\}$
107	$\{0, 14, 21, 47, 53, 59, 85, 92, 106\}$
127	$\{0, 17, 63, 109, 126\}$
131	$\{0, 62, 65, 68, 130\}$
139	$\{0, 68, 69, 70, 138\}$
151	$\{0, 19, 75, 131, 150\}$
167	$\{0, 35, 64, 83, 102, 131, 166\}$

A natural question, which we do not address here, is the following. How big can  $|D(p)|$  be, as a function of  $p$ ?

Theorem 7 implies the following Lucas congruence modulo  $p^3$ .

**Theorem 11.** *Let  $p \geq 5$  and  $n \geq 0$ . If the base- $p$  digits of  $n$  all belong to  $\{0, p-1\}$ , then  $A(n) \equiv 1 \pmod{p^3}$ .*

Experiments do not suggest the existence of any additional Lucas congruences for the Apéry numbers modulo  $p^3$ . We leave this as open question.

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