

FINDING AND EXCLUDING b -ARY MACHIN-TYPE BBP FORMULAE

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ABSTRACT. Constants with formulae of the form treated by D. Bailey, P. Borwein, and S. Plouffe (BBP formulae to a given base b) have interesting computational properties, and there are hints that they should be *normal* numbers, i.e., that their base b digits are randomly distributed. We study a formally limited subset of BBP formulae, which we call Machin-type BBP formulae, for which it is relatively easy to determine whether or not a given constant κ has a Machin-type BBP formula. In particular, given $b \in \mathbb{N}$, $b > 2$, b not a proper power, a b -ary Machin-type BBP arctangent formula for κ is a formula of the form $\kappa = \sum_m a_m \arctan(-b^{-m})$, $a_m \in \mathbb{Q}$, while when $b = 2$ we also allow terms of the form $a_m \arctan(1/(1 - 2^m))$. Of particular interest, we show that π has no Machin-type BBP arctangent formula when $b \neq 2$. To the best of our knowledge, when there is no Machin-type BBP formula for a constant then no BBP formula of any form is known for that constant.

Key words: BBP formulae, Machin-type formulae, arctangents, logarithms, normality, Mersenne primes, Bang's theorem, Zsigmondy's theorem, primitive prime factors, p -adic analysis.

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1. INTRODUCTION

1.1. **Preliminaries.** Given $b \in \mathbb{N}$, $b > 1$, we say that a constant $\kappa \in \mathbb{R}$ has a *BBP formula* to the base b , or a b -ary BBP formula, if

$$(1) \quad \kappa = \sum_{k \geq 0} \frac{p(k)}{q(k)} b^{-k},$$

where $p \in \mathbb{Z}[k]$, $q \in \mathbb{Z}[k]$.

BBP formulae are of interest because, for fixed b , the n th b -ary digit of a number with a BBP formula can be found without computing the previous digits—using only $O(n \ln n)$ operations on numbers with $O(\ln n)$ bits [BBP97]. For example, a BBP formula has been used to compute the quadrillionth bit (10^{15} th bit) in the binary expansion of π [Per00].

There are also recent results that relate BBP formulae to the behavior of a dynamical system, and which offer a “road-map” towards the proof that irrational numbers with BBP formulae must be *normal* in base b , i.e., their base b digits are randomly distributed [BC01]. For example, setting $z = 1/2$ in the Taylor series expansion of $-\ln(1 - z)$ yields the particularly simple binary BBP formula:

$$\ln(2) = \sum_{k \geq 0} \frac{1}{2k + 2} 2^{-k}.$$

In consequence the system with $x_0 := 0$, and

$$x_n := (2x_{n-1} + 1/n) \pmod{1}$$

for $n > 0$ has the property that *if (x_n) is equidistributed in $[0, 1)$ then $\ln 2$ is a normal number base 2.*

While BBP formulae are interesting for these reasons, they are also somewhat mysterious because there are few methods known for finding a formula for a given constant, and even after a formula has been found experimentally it may be difficult to rigorously prove that the formula is valid.

Consider for example, *Catalan’s constant* $G := \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}$ which is not proven irrational. In a series of inspired computations using *polylogarithmic ladders* David Broadhurst has found — and proved — similar identities for constants such as $\zeta(3)$, $\zeta(5)$ and G .

Broadhurst’s quadratic BBP hexadecimal formula for G is explicitly given next.

$$\begin{aligned}
G &= 3 \sum_{k=0}^{\infty} \frac{1}{2 \cdot 16^k} \left\{ \frac{1}{(8k+1)^2} - \frac{1}{(8k+2)^2} + \frac{1}{2(8k+3)^2} - \frac{1}{2^2(8k+5)^2} \right. \\
&\quad \left. + \frac{1}{2^2(8k+6)^2} - \frac{1}{2^3(8k+7)^2} \right\} \\
&- 2 \sum_{k=0}^{\infty} \frac{1}{8 \cdot 16^{3k}} \left\{ \frac{1}{(8k+1)^2} + \frac{1}{2(8k+2)^2} + \frac{1}{2^3(8k+3)^2} - \frac{1}{2^6(8k+5)^2} \right. \\
&\quad \left. - \frac{1}{2^7(8k+6)^2} - \frac{1}{2^9(8k+7)^2} \right\}.
\end{aligned}$$

Given $m \in \mathbb{N}$, a BBP formula to the base b can be rewritten as a BBP formula to the base b^m , since

$$(2) \quad \sum_{k \geq 0} \frac{p(k)}{q(k)} b^{-k} = \sum_{k \geq 0} \left(\sum_{j=0}^{m-1} \frac{p(mk+j)}{b^j q(mk+j)} \right) b^{-mk},$$

and the inner sum can be rewritten as a rational function in k . Although it is a minor abuse of language, we will also refer to formulae to the base b^m as base b , or b -ary, BBP formulae. Under this convention the sum $\sum_k (-1)^k (p(k)/q(k)) b^{-k}$ may also be considered to be a b -ary BBP formulae—a convention that lets one write some “base b ” formulae in a shorter form, although we will avoid doing so in this paper. Unless we mention otherwise, from this point we will assume that b is not a proper power, i.e., that b does not have the form a^n , for any $a \in \mathbb{N}$, $n \in \mathbb{N}$, $n > 1$.

For fixed b , the set of numbers with b -ary BBP formulae is a vector space over \mathbb{Q} . To the best of our knowledge, nearly all research has focused on subspaces of this space generated by elements of the form

$$(3) \quad L(s, b, n, j) := \sum_{k \geq 0} \frac{1}{(nk+j)^s} b^{-k},$$

with $s, n, j \in \mathbb{N}$, $1 \leq j \leq n$. Numbers within these spaces have been called *polylogarithmic*—a term which we will reserve for \mathbb{Q} -linear combinations of $L(s, b, n, j)$ in which only j is allowed to vary.

In his *Compendium* [Bai00], Bailey catalogues many polylogarithmic constants. Bailey uses the notation

$$(4) \quad P(s, b, n, A) := \sum_{k \geq 0} b^{-k} \sum_{j=1}^n \frac{a_j}{(nk+j)^s},$$

where $A = [a_1, \dots, a_n] \in \mathbb{Z}^n$. In terms of our $L(s, b, n, j)$ we have

$$(5) \quad P(s, b, n, A) = \sum_{j=1}^n a_j L(s, b, n, j).$$

Let $\text{span}\{\alpha_k\}$ denote the vector space over \mathbb{Q} spanned by the set $\{\alpha_k\}$. The spaces of polylogarithmic constants explored by Bailey have the form

$$\text{span}\{P(s, b, n, A) : A \in \mathbb{Z}^n\} = \text{span}\{L(s, b, n, j) : 1 \leq j \leq n\}$$

with s, b, n fixed, and with b allowed to be a power, such as 2^4 . Bailey has found many “interesting” constants κ in these spaces by computing κ and a table of $L(s, b, n, j)$, $1 \leq j \leq n$, to high precision; and then using the PSLQ integer relation algorithm [FBA99] to find $a \in \mathbb{Z}$, $A \in \mathbb{Z}^n$ such that $a\kappa = P(s, b, n, A)$.

1.2. Our goals. In this paper we focus our attention on *degree one*, or “logarithmic”, BBP formulae, i.e., those where $s = 1$ in (4). We further restrict ourselves to formulae of a special form which we call *Machin-type*. Roughly speaking, we say that κ has a Machin-type BBP formula to the base b (or κ has a b -ary Machin-type BBP formula) to mean that κ can be written either as a \mathbb{Q} -linear combination of real parts of logarithms, or of imaginary parts of logarithms, where the logarithms are chosen so as to yield a BBP formula to the base b .

The numbers whose logarithms we consider all lie in the multiplicative group $\mathbb{Q}[i]^\times$. Knowledge of how numbers factor into primes over $\mathbb{Z}[i]$ (the Gaussian integers) or over \mathbb{Z} serves as a tool both for finding Machin-type BBP formulae and for showing that no such formula can exist. Despite the restricted nature of Machin-type BBP formulae, to the best of our knowledge when we can show that there is no b -ary Machin-type formula for a constant then no b -ary BBP formula of any form is known for that constant.

2. MACHIN-TYPE BBP FORMULAE FOR ARCTANGENTS

2.1. A brief survey of Machin-type formulae. The original Machin formula is the identity

$$(6) \quad \pi/4 = 4 \arctan(1/5) - \arctan(1/239) \quad (\text{Machin, 1706}).$$

Machin used this formula to compute 100 digits of π . Similar *Machin-type formulae* for π , i.e., formulae which express π as a \mathbb{Z} -linear combination of arctangents, have been used in most other extended computations of π until around 1980 and a few million digits. In recent years it has generally been believed that quite different formulae for π , such as the “AGM formula”, are better suited for the computation of π ; they are surely of lower operational complexity, but involve full precision intermediate calculation, and were used beyond 200 billion digits. (See [BB98, §11.1] for some history on π computations.) However, in December 2002, Yasumasa Kanada announced the record computation of 1.24 trillion decimal digits of π , using

the identities

$$(7) \quad \pi = 48 \arctan(1/49) + 128 \arctan(1/57) - 20 \arctan(1/239) \\ + 48 \arctan(1/110443)$$

$$(8) \quad \pi = 176 \arctan(1/57) + 28 \arctan(1/239) - 48 \arctan(1/682) \\ + 96 \arctan(1/12943).$$

Indeed, for the size of computation being undertaken full precision floating point computations are again impracticable.

One way to “discover” Machin’s formula (6) is to observe that

$$(9) \quad \arctan(y/x) \equiv \Im \ln(x + iy) \pmod{\pi}.$$

(We will give our choice of branch-cut for $\arctan(\rho)$ and $\ln(z)$ below.) Equation (9), and the fact that $(5 + i)^4(239 + i)^{-1} = 2 + 2i$ imply

$$(10) \quad \pi/4 = \arctan(1) \equiv 4 \arctan(1/5) - \arctan(1/239) \pmod{\pi}.$$

True equality of the two sides of the congruence is easily verified numerically, by computing both sides to sufficient precision to ensure that they differ by less than π . Similarly, the process of verifying Equations (7) and (8) can be reduced to verifying that the products

$$(49 + i)^{48}(57 + i)^{128}(239 + i)^{-20}(110443 + i)^{48}$$

and

$$(57 + i)^{176}(239 + i)^{28}(682 + i)^{-48}(12943 + i)^{96}$$

both yield negative rational numbers.

This same technique of formulating a question about arctangents in terms of properties of $\mathbb{Z}[i]$ was used by Størmer in 1897 to solve a problem of Gravé. Gravé’s problem comprises that there are only four non-trivial integral solutions to

$$m \arctan(1/u) + n \arctan(1/v) = k\pi/4,$$

namely Machin’s formula (6), and

$$(11) \quad \pi/4 = \arctan(1/2) + \arctan(1/3) \quad (\text{Euler, 1738})$$

$$(12) \quad \pi/4 = 2 \arctan(1/2) - \arctan(1/7) \quad (\text{Hermann, 1706})$$

$$(13) \quad \pi/4 = 2 \arctan(1/3) + \arctan(1/7) \quad (\text{Hutton, 1776}).$$

Further information on Størmer’s solution to can be found in [BB98, §11.1, Exercise 6], or, more completely, in [Rib94, §A.12].

2.2. Notational conventions. Throughout this paper $\arctan(\rho)$ denotes the principal branch of the arctangent function, defined so that $-\pi/2 < \arctan(\rho) < \pi/2$ for $\rho \in \mathbb{R}$. We also allow the case $\rho = \infty$, and define $\arctan(\infty) := \pi/2$ and also define $\tan(\pm\pi/2) := \infty$. Given $\rho \neq 0$ we define $\rho/0 := \infty$, regardless of the sign of ρ . Similarly, $\ln(z)$ denotes the principal branch of the logarithm function, defined so that $\ln(z) = \ln(|z|) + i\theta$ satisfies $-\pi < \theta \leq \pi$. In other words $\theta = \Im \ln(z)$ satisfies $e^{i\theta} = z/|z|$, $-\pi < \theta \leq \pi$.

(The function $\Im \ln(z)$ is also known as the *argument* of z , $\arg(z)$.) Given $x, y \in \mathbb{R}$, our definitions of $\ln(z)$ and $\arctan(\rho)$ ensure that

$$\arctan(y/x) = \Im \ln(x + iy) = \frac{1}{2} \ln \left(\frac{x + iy}{x - iy} \right)$$

provided $x > 0$. More generally, under our conventions we always have $\arctan(y/x) \equiv \Im \ln(x + iy) \pmod{\pi}$, including the case $x = 0, y \neq 0$.

2.3. Using group homomorphisms. As in our derivation of Machin's formula in Section 2.1, we will use some basic group theory to guide us in our search for BBP formulae. We start with a set $\{\kappa_1, \kappa_2, \dots\}$ of constants with known BBP formulae, and a constant κ for which we wish to determine a BBP formula. Provided $\kappa \in \text{span}\{\kappa_1, \kappa_2, \dots\}$, finding a BBP formula for κ in terms of the formulae for κ_j is equivalent to finding a \mathbb{Q} -linear relationship of the form

$$\kappa = \sum_j a_j \kappa_j,$$

or, rearranging and multiplying through by a common denominator, this is equivalent to finding a \mathbb{Z} -linear relationship of the form

$$(14) \quad n\kappa + \sum_j n_j \kappa_j = 0.$$

In other words, we wish to determine if there is an $n \in \mathbb{Z}$ for which $n\kappa$ lies in the additive Abelian group G generated by $\{\kappa_1, \kappa_2, \dots\}$. Although we have little knowledge about G , we can choose a group homomorphism $f: G \rightarrow H$ where the *target group* H is *well understood*. (Note that f need not be surjective—in our applications we will typically have $\text{img } f \subsetneq H$.)

Given the homomorphism f , we are lead to finding a relationship of the form

$$(15) \quad \begin{aligned} n f(\kappa) + \sum_j n_j f(\kappa_j) &= 0 \quad \text{or,} \\ f(\kappa)^n \prod_j f(\kappa_j)^{n_j} &= 1, \end{aligned}$$

according to whether H is an additive group or an Abelian multiplicative group. If there is no solution to (15) then there is no solution to Equation (14), and κ cannot be represented in terms of $\{\kappa_1, \kappa_2, \dots\}$. On the other hand, a solution to (15) does not ensure a solution to (14), but only ensures that

$$(16) \quad n\kappa + \sum_j n_j \kappa_j = \kappa_0$$

for some $\kappa_0 \in \ker f$. Thus, to verify that κ can be represented in terms of $\{\kappa_1, \kappa_2, \dots\}$, it suffices to solve (15) and to verify either that $\ker f = \{0\}$ or to further examine the left side of (16) (e.g., with a numerical test) to verify that $\kappa_0 = 0$.

In our search for arctangent formulae there are two, nearly equivalent, choices of target group that seem convenient, and we will use both. In some cases we will identify an angle $\theta \in \mathbb{R}$ with the line of slope $\tan(\theta)$. Writing members of group quotients as explicit cosets, the corresponding homomorphism is essentially $f: \mathbb{R} \rightarrow \mathbb{C}^\times/\mathbb{R}^\times$, $f(\theta) = e^{i\theta}\mathbb{R}^\times$. We will call $\mathbb{C}^\times/\mathbb{R}^\times$ the *group of slopes*. More precisely, with $f(\theta)$ as above, we will be using the homomorphism $f|_G$, the restriction of f to G . Since we are working with $G < \mathbb{R}$ generated by elements of the form $\arctan(\rho)$, $\rho \in \mathbb{Q}$ we may take $H = \mathbb{Q}[i]^\times\mathbb{R}^\times/\mathbb{R}^\times \cong \mathbb{Q}[i]^\times/\mathbb{Q}^\times$. The group $\mathbb{Q}[i]^\times/\mathbb{Q}^\times$ has a rich number-theoretical structure which will guide us in our search for BBP formulae.

In other cases we will identify an angle θ with the directed ray $e^{i\theta}\mathbb{R}_+^\times$, via the homomorphism $f: \mathbb{R} \rightarrow \mathbb{C}/\mathbb{R}_+^\times$, $f(\theta) = e^{i\theta}\mathbb{R}_+^\times$, where \mathbb{R}_+^\times is the multiplicative group of positive real numbers. By identifying the ray $e^{i\theta}\mathbb{R}_+^\times$ with the point $e^{i\theta}$ we see that $\mathbb{C}/\mathbb{R}_+^\times$ is isomorphic to the *unit circle* group $\mathbb{S} := \{z \in \mathbb{C} : |z| = 1\}$. As before, in this case we may take the target group to be $H = \mathbb{Q}[i]^\times\mathbb{R}_+^\times/\mathbb{R}_+^\times \cong \mathbb{Q}[i]^\times/\mathbb{Q}_+^\times$.

Remark. Our group of slopes, $\mathbb{C}^\times/\mathbb{R}^\times$, can be considered as the real projective line $\mathbb{P}_\mathbb{R}$, endowed with a group structure. In more detail,

$$\mathbb{P}_\mathbb{R} := \{(y, x) \in \mathbb{R} \times \mathbb{R} : (y, x) \neq (0, 0)\},$$

under the equivalence relation $(y, x) \sim (\lambda y, \lambda x)$ for all $\lambda \neq 0$, $\lambda \in \mathbb{R}$. Writing y/x to denote the equivalence class of (y, x) , we can embed $\mathbb{R} \subset \mathbb{P}_\mathbb{R}$ under the map $y \mapsto y/1$. Of course $1/0$ denotes ∞ : the *point at infinity*. In some earlier research notes we have written $(y_1/x_1) \otimes (y_2/x_2)$ for multiplication in this group, where

$$\frac{y_1}{x_1} \otimes \frac{y_2}{x_2} \sim \frac{y_1x_2 + y_2x_1}{x_1x_2 - y_1y_2}.$$

With this notation, $\mathbb{P}_\mathbb{R}$ has identity $0/1$, and the (multiplicative) inverse of y/x is $-y/x$. \square

2.4. Generators for Machin-type BBP arctangent formulae. We now describe our *Machin-type BBP generators* and the resulting formulae. Given b not a proper power, $b > 2$, these are generators of the form

$$\begin{aligned} \arctan(-b^{-m}) &= \Im \ln(1 - ib^{-m}) = -b^{-m} \sum_{k \geq 0} \frac{(-1)^k}{2k+1} b^{-2mk} \\ &= b^{-3m} P(1, b^{4m}, 4, [-b^{2m}, 0, 1, 0]). \end{aligned}$$

The series expansion for $\arctan(x/(1+x))$ yields a binary BBP formula when $x = \pm 2^{-m}$. Thus, when $b = 2$ we use additional generators of the form $\arctan(1/(1-2^m)) = \Im \ln(1 - (1+i)2^{-m})$. We call these generators *Aurifeuillian* because of their similarity to the Aurifeuillian logarithmic generators defined in Section 3. Such factorizations were discovered by Aurifeuille and Le Lasseur but first described in print in 1878 by Lucas (see

page 126 of [Wil98]). The BBP formulae for these Aurifeuillian generators are given in Appendix A.

Definition 1. Given $\kappa \in \mathbb{R}$, $2 \leq b \in \mathbb{N}$, b not a proper power, we say that κ has a \mathbb{Z} -linear or \mathbb{Q} -linear *Machin-type BBP arctangent formula* to the base b if and only if κ can be written as a \mathbb{Z} -linear or \mathbb{Q} -linear combination (respectively) of generators of the form described in the previous paragraph. A non-Aurifeuillian formula is one which does not use Aurifeuillian generators. (Note that all formulae are non-Aurifeuillian when $b > 2$.) More briefly, when κ has a \mathbb{Q} -linear formula we will say that κ has a b -ary Machin-type BBP arctangent formula. ■

Remarks. Although our Machin-type BBP formulae are in one sense more restricted than the formulae considered by Bailey, at first glance they also appear to be more general, in that we allow linear combinations of $P(1, b^m, n, \dots)$ where both m and n may vary. However, in Appendix B we will show that any Machin-type BBP formula may be reduced to Bailey's form.

We will call the generators of Definition 1 the *minimal set* of arctangent generators, although for fixed b this set is not necessarily linearly independent. When $b = 2$ it is sometimes convenient when doing hand computations to use all elements of the form $\Im \ln(1 \pm (1+i)2^{-m}) = \arctan(1/(1 \pm 2^m))$ as generators. Note however that both our minimal set of generators and the *full set* described above span the same space, as can easily be shown using the identity

$$\Im \ln(1 + (1+i)2^{-m}) = \Im \ln(1 - i2^{1-2m}) - \Im \ln(1 - (1+i)2^{-m}).$$

Note that $(1 - ib^{-m})\mathbb{R}^\times = (b^m - i)\mathbb{R}^\times$. In other words, both sides of the equality represent the same element in our group of slopes. Along the same lines we have $\Im \ln(1 - ib^{-m}) = \Im \ln(b^m - i)$. Since it is generally easier to work with elements of $\mathbb{Z}[i]^\times$ instead of $\mathbb{Q}[i]^\times$, we will often prefer to write $(b^m - i)\mathbb{R}^\times$ instead of $(1 - ib^{-m})\mathbb{R}^\times$. Similarly, we will often prefer $(2^m - 1 - i)\mathbb{R}^\times$ to $(1 - (1+i)2^{-m})\mathbb{R}^\times$ and we will prefer to write the inverse of $(x + iy)\mathbb{R}^\times$ as $(x - iy)\mathbb{R}^\times$. (We will follow the corresponding practice when working with elements of $\mathbb{C}^\times/\mathbb{R}_+^\times$, with \mathbb{R}_+^\times replacing the role of \mathbb{R}^\times .)

□

2.5. Finding Machin-type BBP arctangent formulae. With these preliminary remarks out of the way, we almost immediately find a binary Machin-type BBP formulae for $\pi/4$ by noting that

$$\begin{aligned} \pi/4 &= -\Im \ln(1 - i) = -\arctan(-1) \\ (17) \quad &= 2^{-4}P(1, 2^4, 8, [8, 8, 4, 0, -2, -2, -1, 0]). \end{aligned}$$

(This formula seems to have first been observed by Helaman Ferguson. See [Bai00, Equation (13)] and also [FBA99, page 352].)

Further binary formulae for $\pi/4$ can be found in much the same way as in our development of Formula (10), and as in Størmer's solution to Grave's

problem, by looking for products of the form

$$(18) \quad z := \prod_j (2^{m_j} - i)^{n_j} \prod_j (2^{m_j} - 1 - i)^{n_j}$$

which yield $z \in (1+i)\mathbb{R}_+^\times$, and thus $\Im \ln(z) \equiv \pi/4 \pmod{2\pi}$. More generally, when looking for \mathbb{Z} -linear formulae for some multiple of π , we would consider products of the form (18) yielding $z \in (1+i)^n \mathbb{R}_+^\times$, and thus $\Im \ln(z) \equiv n\pi/4 \pmod{2\pi}$. Note that when $n \equiv 0 \pmod{8}$ it is possible that $\Im \ln(z) = 0$.

A hand search for additional formulae soon reveals that

$$(19) \quad (2-i)(3-i) = 5 - 5i,$$

$$(20) \quad (2-i)^2(7+i) = 25 - 25i,$$

$$(21) \quad (3-i)^2(7-i) = 50 - 50i,$$

corresponding to the solutions (11)–(13) of Gravé’s problem. Since each factor on the left hand sides has the one of the desired forms $2^m - i$ or $2^m - 1 - i$ for some m we see that (11), (12), and (13) all yield binary Machin-type BBP arctangent formulae for $\pi/4$.

Similarly, a hand search gives binary Machin-type BBP arctangent formulae for $\arctan(1/6)$, $\arctan(5/6)$, and $\arctan(1/11)$ via the factorizations

$$6 + i = (5 + i)(31 - i)/26,$$

$$6 + 5i = (1 + i)(5 - i)(9 + i)(255 - i)/2132,$$

$$11 + i = (1 + i)(6 - 5i), \text{ and then factor } (6 - 5i) \text{ as } \overline{6 + 5i}.$$

These factorizations give formulae in terms of our full set of generators:

$$\arctan(1/6) = \arctan(1/5) - \arctan(1/31)$$

and

$$\arctan(5/6) = \arctan(1) - \arctan(1/5) + \arctan(1/9) - \arctan(1/255)$$

while

$$\arctan(1/11) = \arctan(1) - \arctan(5/6).$$

No formulae for these three arctangents are listed in Bailey’s *Compendium* [Bai00, §3]. However, the above results show that $\arctan(1/6)$, $\arctan(5/6)$ and $\arctan(1/11)$ do indeed admit binary Machin-type BBP formulae. (The process of converting such formulae to Bailey’s form is detailed in Appendix B.) Among the values missing in Bailey’s list, the first arctangent for which we have been unable to find a binary Machin-type BBP formula is $\arctan(2/7)$.

We can make the search for arctangent formulae more systematic by examining how $2^m - i$ and $2^m - 1 - i$ factor into primes over $\mathbb{Z}[i]$. Since primes in $\mathbb{Z}[i]$ are only defined up to a factor of i^n , we will always take a “canonical” factorization of $z \in \mathbb{Z}[i]$, of the form

$$(22) \quad z = i^n \prod_j \mathfrak{p}_j^{n_j},$$

where \mathfrak{p}_j runs through some subset of the primes of $\mathbb{Z}[i]$, and where for each prime \mathfrak{p} we require that $\Re \mathfrak{p} > 0$, $-\Re \mathfrak{p} < \Im \mathfrak{p} \leq \Re \mathfrak{p}$, so that $-\pi/4 < \Im \ln \mathfrak{p} \leq \pi/4$. These conditions uniquely define $n \pmod{4}$, where n is the exponent appearing in i^n . To make n completely unique, we further require that $-1 \leq n \leq 2$. The factorization of $z \in \mathbb{Z}[i]$ can easily be found in Maple using the `GaussInt` package, or in Mathematica using `FactorInteger[z, GaussianIntegers→True]`. (However, in both cases additional work is needed to get a canonical factorization in our sense.) Since, given $z, w \in \mathbb{C}$, $\Im \ln(zw) \equiv \Im \ln(z) + \Im \ln(w) \pmod{2\pi}$, the factorization (22) gives

$$\Im \ln(z) \equiv n\pi/2 + \sum_j n_j \Im \ln \mathfrak{p}_j \pmod{2\pi}.$$

In many cases, this equivalence modulo 2π corresponds to true equality, but the example $z = (2+i)^{12} = 11753 - 10296i$, $\Im \ln(z) \approx -0.7194$ while $12\Im \ln(2+i) \approx 5.5638$, demonstrates that this is not always true.

To illustrate, we use this technique to more systematically find formulae for π . Let $\beta_m := \Im \ln(2^m - i)$ and $\alpha_m := \Im \ln(2^m - i - 1)$ denote our binary Machin-type BBP arctangent generators. For the first few generators, factoring the arguments $2^m - i$ of $\Im \ln(\dots)$ into primes over $\mathbb{Z}[i]$ gives

$$(23) \quad 2^1 - i = 2 - i$$

$$(24) \quad 2^2 - i = 4 - i$$

$$(25) \quad 2^3 - i = (2+i)(3-2i),$$

while for the Aurifeuillian arguments $2^m - 1 - i$ we find

$$(26) \quad 2^1 - 1 - i = 1 - i$$

$$(27) \quad 2^2 - 1 - i = i^{-1}(1+i)(2+i)$$

$$(28) \quad 2^3 - 1 - i = (1+i)(2-i)^2.$$

Using $\Im \ln(i) = \pi/2$, $\Im \ln(1+i) = \pi/2$, $\Im \ln(\bar{\mathfrak{p}}) = -\Im \ln(\mathfrak{p})$; and checking that we have the correct congruence class modulo 2π , the factorizations (23) through (25) give

$$(29) \quad \beta_1 = -\Im \ln(2+i)$$

$$(30) \quad \beta_2 = -\Im \ln(4+i)$$

$$(31) \quad \beta_3 = \Im \ln(2+i) - \Im \ln(3+2i),$$

while, by (26) through (28), our Aurifeuillian generators decompose as

$$(32) \quad \alpha_1 = -\pi/4$$

$$(33) \quad \alpha_2 = -\pi/4 + \Im \ln(2+i)$$

$$(34) \quad \alpha_3 = \pi/4 - 2\Im \ln(2+i).$$

(The presence of $\pi/4$ in our Aurifeuillian generators could have been predicted from the fact that $1+i \mid x+iy$ when x^2+y^2 is even.)

With these decompositions (essentially a change of basis in our vector space over \mathbb{Q}), we can easily spot \mathbb{Z} -linear dependencies between β_1 , α_1 , α_2 , and α_3 . From these dependencies we once again get formulae for $\pi/4$ corresponding to Equations (19)–(21). Equivalently, we get two linearly independent zero relations such as

$$(35) \quad \alpha_1 + \alpha_3 - 2\beta_1 = 0$$

$$(36) \quad \alpha_1 - 2\alpha_2 - \alpha_3 = 0.$$

2.6. Exclusion criteria for Machin-type BBP arctangent formulae.

The type of reasoning used above can also be used to exclude the possibility of a Machin-type BBP formula, as illustrated in Theorems 1 and 2 below. In the following discussion $\nu_b(p)$ denotes the order of b in the multiplicative group modulo a prime p . Given $z \in \mathbb{Q}$, $\text{ord}_p(z)$ denotes the usual p -adic order of z , which can be defined by stating that $\text{ord}_p(p) = 1$, $\text{ord}_p(q) = 0$ for any prime $q \neq p$, and $\text{ord}_p(zw) = \text{ord}_p(z) + \text{ord}_p(w)$. (Note that $\text{ord}_p: \mathbb{Q}^\times \rightarrow \mathbb{Z}$ is a group homomorphism. For more information on p -adic orders, see, for example, the book by Koblitz [Kob84].)

Theorem 1. *Given $2 \leq b \in \mathbb{N}$, b not a proper power, and given $x \in \mathbb{Z}$, $y \in \mathbb{Z}$, suppose there is a prime $p \equiv 1 \pmod{4}$ with $\text{ord}_p(x^2 + y^2)$ odd, such that either $p \mid b$; or $p \nmid b$, $4 \nmid \nu_b(p)$. Then $\arctan(y/x)$ does not have a \mathbb{Z} -linear Machin-type BBP arctangent formula to the base b .*

Before giving the proof we remark that we cannot have $\text{ord}_p(x^2 + y^2)$ odd when $p \equiv 3 \pmod{4}$.

Proof. We first consider the simpler case where $b > 2$, so that there are no Aurifeuillian generators to consider. In this case, if there were a formula for $\arctan(y/x)$, we would have

$$(37) \quad (x + iy)\mathbb{R}^\times = \prod_j (b^{m_j} - i)^{n_j} \mathbb{R}^\times,$$

$m_j \in \mathbb{N}$, $n_j \in \mathbb{Z}$. Since a real-valued product of elements of $\mathbb{Q}[i]^\times$ must lie in \mathbb{Q}^\times , we conclude from Equation (37) that

$$(38) \quad (x + iy) \prod_j (b^{m_j} - i)^{-n_j} = M/N \in \mathbb{Q}^\times.$$

Taking norms (multiplying each expression by its complex conjugate) in (38) yields

$$(x^2 + y^2) \prod_j (b^{2m_j} + 1)^{-n_j} = M^2/N^2.$$

Since $\text{ord}_p(x^2 + y^2)$ is assumed odd but $\text{ord}_p(M^2/N^2)$ must be even, we must have $p \mid b^{2m_j} + 1$ for at least one j . Clearly this cannot happen if $p \mid b$. Now assuming that $p \nmid b$, $4 \nmid \nu_b(p)$, and letting $m = m_j$ we find

$$(39) \quad b^{2m} \equiv -1 \pmod{p},$$

and so $b^{4m} \equiv 1 \pmod{p}$. Thus we conclude that $\nu_b(p) \mid 4m$. But $4 \nmid \nu_b(p)$, so $\nu_b(p) \mid 2m$, giving $b^{2m} \equiv 1 \pmod{p}$, contradicting (39).

The argument when $b = 2$ is similar. Note that we cannot have $p \mid b$ in this case. Now, if there were a formula for $\arctan(y/x)$, we would have an identity of the form

$$(40) \quad (x + iy)\mathbb{R}^\times = \prod_j (2^{m_j} - i)^{n_j} \prod_j (2^{m_j} - (1 + i))^{n_j} \mathbb{R}^\times.$$

Arguing as before, and taking norms, we conclude that

$$(x^2 + y^2) \prod_j (2^{2m_j} + 1)^{-n_j} \prod_j (2^{m_j} - (1 + i))^{-n_j} (2^{m_j} - (1 - i))^{-n_j} = M^2/N^2.$$

Since $p \equiv 1 \pmod{4}$, there is an $I \in \mathbb{Z}$ satisfying $I^2 \equiv -1$. As before, since $\text{ord}_p(x^2 + y^2)$ is assumed odd but $\text{ord}_p(M^2/N^2)$ must be even, at least one of $p \mid 2^{2m_j} + 1$; $p \mid 2^{m_j} - (1 + I)$; or $p \mid 2^{m_j} - (1 - I)$ must hold. The first case immediately leads to a contradiction, as when $b > 2$. The latter two cases give $2^{m_j} \equiv 1 \pm I \pmod{p}$. Raising both sides to the fourth power gives $2^{4m_j} \equiv -4 \pmod{p}$, so, letting $m = 2m_j - 1$, we have $2^{2m} \equiv -1 \pmod{p}$, which again leads to a contradiction, as when $b > 2$. \blacksquare

Example 1. Using $p = 5$ and $\text{ord}_5(2^2 + 1^2) = 1$ in Theorem 1, we conclude that there is no b -ary \mathbb{Z} -linear Machin-type BBP formulae for $\arctan(1/2)$ when $5 \mid b$. Similarly, using $p = 13$ and $\text{ord}_{13}(5^2 + 1^2) = 1$, we conclude that there is no b -ary \mathbb{Z} -linear Machin-type BBP formulae for $\arctan(1/5)$ when $13 \mid b$. \square

Example 2. Using the second exclusion criterion of Theorem 1, with $p = 13$ and noting $3^2 + 2^2 = 13$ and $\nu_3(13) = 3$, we conclude that $\arctan(2/3)$ has no 3-ary \mathbb{Z} -linear Machin-type BBP arctangent formula. More generally, no odd multiple of $\arctan(2/3)$ has a 3-ary \mathbb{Z} -linear Machin-type BBP arctangent formula.

Similarly, with $b = 2$ and $p = 73$, noting that $8^2 + 3^2 = 73$, we conclude that $\arctan(3/8)$ has no binary \mathbb{Z} -linear Machin-type BBP arctangent formula, as $\nu_2(73) = 9$. Correspondingly with $b = 2$ and $p = 89$, noting that $8^2 + 5^2 = 89$, we conclude that $\arctan(5/8)$ has no binary \mathbb{Z} -linear Machin-type BBP formula. Similarly, $\arctan(5/11)$ has no binary formula, since $146 = 2 \cdot 73$. Also $9/16$ yields 337 with group order 21, and $11/16$ yields 445 which is divisible by 89 with group order 11. (See also Appendix D on density of arctans with or without Machin-type formulae.)

We have ruled out formulae for $3/8$ and $5/8$. Every other fraction with denominator less than 10 has a known binary linear Machin-type formula, except for $2/7, 4/9, 5/9$, which are presently in limbo. In these three cases the exclusion criterion of Theorem 1 fails. We return to these orphans in Example 3. \square

We get a stronger exclusion criterion for Machin-type BBP arctangent formulae by looking at how $(x + iy)$ factors in $Z[i]$:

Definition 2. Given $z \in \mathbb{Q}[i]$, and a rational prime $p \equiv 1 \pmod{4}$, let $\vartheta_p(z)$ denote $\text{ord}_{\mathfrak{p}}(z) - \text{ord}_{\bar{\mathfrak{p}}}(z)$, where \mathfrak{p} and $\bar{\mathfrak{p}}$ are the two conjugate Gaussian primes dividing p , and where we require $0 < \Im \mathfrak{p} < \Re \mathfrak{p}$ to make the definition of ϑ_p unambiguous. \blacksquare

Note that

$$(41) \quad \vartheta_p(zw) = \vartheta_p(z) + \vartheta_p(w).$$

It's also easy to see that $w \in \mathbb{Q}^\times$ implies that $\vartheta_p(w) = 0$, so it makes sense to define $\vartheta_p(z\mathbb{Q}^\times) := \vartheta_p(z)$.

Theorem 2. Given $2 \leq b \in \mathbb{N}$, b not a proper power, and given $x \in \mathbb{N}$, $y \in \mathbb{N}$, suppose there is a prime p not dividing b , with $p \equiv 1 \pmod{4}$ and $\vartheta_p(x + iy) \neq 0$. Suppose either (a) $4 \nmid \nu_b(p)$, or (b) the prime $p \equiv 1 \pmod{4}$, such that $4 \mid \nu_b(p)$, is unique, and there is a prime $q \equiv 1 \pmod{4}$ with $\vartheta_q(x + iy) = 0$ and $\nu_b(p) = \nu_b(q)$.

Then in case (a) $\arctan(y/x)$ does not have a \mathbb{Q} -linear Machin-type BBP arctangent formula to the base b ; and in case (b) $\arctan(y/x)$ has no non-Aurifeuillian \mathbb{Q} -linear Machin-type BBP arctangent formula to the base b .

Proof. Our proof of (a) is similar to the proof of Theorem 1. Again, we first consider the case $b > 2$, where there are no Aurifeuillian generators to consider. In this case, if there were a \mathbb{Q} -linear Machin-type BBP formula for $\arctan(y/x)$ then for some $n \in \mathbb{Z}$, $n \neq 0$ we would have

$$(x + iy)^n \prod_j (b^{m_j} - i)^{-n_j} = M/N \in \mathbb{Q}^\times.$$

Our assumption that $\vartheta_p(x + iy) \neq 0$ implies $\vartheta_p((x + iy)^n) \neq 0$, which together with $\vartheta_p(M/N) = 0$ implies $\vartheta_p(b^{m_j} - i) \neq 0$ for at least one j . So, at least one of \mathfrak{p} , $\bar{\mathfrak{p}}$ divides $b^{m_j} - i$. Thus, letting $m = m_j$, assume that $\mathfrak{p} \mid b^m - i$. (The argument when $\bar{\mathfrak{p}} \mid b^m - i$ is nearly identical.) Since $\mathfrak{p} \mid b^m - i$ we have $\bar{\mathfrak{p}} \mid b^m + i$, and thus $\mathfrak{p}\bar{\mathfrak{p}} \mid b^{2m} + 1$. In other words, $b^{2m} \equiv -1 \pmod{p}$, which gives a contradiction, as in the proof of Theorem 1.

We now consider the case when $b = 2$. In this case a formula for $\arctan(y/x)$ would imply that we had an identity of the form

$$(x + iy)\mathbb{R}^\times = \prod_j (2^{m_j} - i)^{n_j} \prod_j (2^{m_j} - (1 + i))^{n_j} \mathbb{R}^\times.$$

Our assumption that $\vartheta_p(x + iy) \neq 0$ leads us to conclude that at least one of \mathfrak{p} , $\bar{\mathfrak{p}}$ divides at least one of $2^{m_j} - i$ or $2^{m_j} - (1 + i)$ for some j . Again, without loss of generality, assume that \mathfrak{p} is the divisor. If $\mathfrak{p} \mid 2^{m_j} - i$ we get a contradiction, as when $b > 2$. If $\mathfrak{p} \mid 2^{m_j} - (1 + i)$ then, letting $m = 2m_j - 1$, it follows that $b^{2m} \equiv -1 \pmod{p}$, which again gives a contradiction.

We defer the proof of part (b) until Section 3.4. \blacksquare

Example 3. Continuing Example 2, looking for a ternary arctangent formula for $\arctan(2/3)$, we use $p = 13$ in Theorem 2 (a), still noting that $\nu_3(13) = 3$, and using $\vartheta_{13}(3 + 2i) = 1$, to conclude that $\arctan(2/3)$ has no 3-ary \mathbb{Q} -linear Machin-type BBP arctangent formula. This can be applied to various of the other fractions in Example 2 such as $3/8, 5/8, 5/11, 9/16$, and $11/16$.

We illustrate Theorem 2 (b), as follows. Firstly it shows us that $\arctan(1/4)$ has no 3-ary \mathbb{Q} -linear Machin-type BBP arctangent, since $\nu_3(17) = \nu_3(193) = 16$. Correspondingly, we may rule out Aurifeuillian binary formulae for arctangents of the fractions $2/7, 4/9$ and $5/9$. Indeed $2^2 + 7^2 = 53, 5^2 + 9^2 = 53 \cdot 2$ and $\nu_2(53) = \nu_2(157) = 52$. Similarly, $4^2 + 9^2 = 97$ and $\nu_2(97) = \nu_2(673) = 48$. \square

We can clarify the meaning of ϑ_p by extending its definition to cover all prime p . Given $z \in \mathbb{Q}[i]^\times$ we can write $z\mathbb{R}^\times = z_0\mathbb{R}^\times$ with $z_0 \in \mathbb{Z}[i]$, and so that z_0 factors over $\mathbb{Z}[i]$ as

$$(42) \quad z_0 = (1 + i)^k \prod_{\substack{p \equiv 1 \pmod{4} \\ p = \mathfrak{p}\bar{\mathfrak{p}}}} \mathfrak{p}^{\text{ord}_{\mathfrak{p}}(z)} \bar{\mathfrak{p}}^{\text{ord}_{\bar{\mathfrak{p}}}(z)},$$

with $0 \leq k < 8$ and with $0 < \Im \mathfrak{p} < \Re \mathfrak{p}$. (When $z \in \mathbb{Z}[i]$ we have $k \equiv 2n + \text{ord}_{1+i}(z) \pmod{8}$, where n is defined by the canonical factorization of z defined following Equation (22). Similarly, when $z \in \mathbb{Q}[i]$, we can compute $k \pmod{8}$ from the canonical factorizations of the numerator and denominator of z .) Now, let $\vartheta_2(z) := k$, where k is given by Equation (42). (Note that $\vartheta_2(zw) \equiv \vartheta_2(z) + \vartheta_2(w) \pmod{8}$.)

With this extended definition of ϑ_p , we have

$$\Im \ln(z) \equiv \vartheta_2(z) \Im \ln(1 + i) + \sum_{p \equiv 1 \pmod{4}} \vartheta_p(z) \Im \ln(\mathfrak{p}) \pmod{2\pi}.$$

Thus, $\vartheta_p(z)$ measures the contribution to $\Im \ln(z)$ which can be attributed to $1 + i$ (the single Gaussian prime dividing 2) and to the Gaussian primes $\mathfrak{p} \mid p, \bar{\mathfrak{p}} \mid p, p \equiv 1 \pmod{4}$. For completeness, we will define $\vartheta_p(z) := 0$ when $p \equiv 3 \pmod{4}$, since these primes do not factor further over $\mathbb{Z}[i]$ and thus contribute nothing to $\Im \ln(z)$.

Given a finite set of generators of the form $\Im \ln(z)$, $z \in \mathbb{Q}[i]$, we could, in principle, use values of ϑ_p to automate the process which we informally used to spot the zero relations (35) and (36) given earlier. For each generator of the form $\Im \ln(z)$ we would compute a vector of $\vartheta_p(z)$, indexed by p , where p runs through a finite subset of $\{2\} \cup \{p \text{ prime} : p \equiv 1 \pmod{4}\}$. (The ϑ_2 component of the vectors should be treated as an element of $\mathbb{Z}/(8\mathbb{Z})$.) Given these vectors, the process of finding possible linear dependencies could be automated by using the algorithms described in [Coh93, §2.4] for analyzing \mathbb{Z} -modules, (i.e., Abelian groups). The dependencies found this way are only “possible” dependencies, both because knowledge of $\vartheta_p(z)$ for all p only determines $\Im \ln z \pmod{2\pi}$, and because we may choose to restrict

ourself to a small subset of primes, and thus will get less than complete information about how the various z factor in $\mathbb{Z}[i]$. (Consider the problem of completely factoring $2^{1001} - i$ over $\mathbb{Z}[i]$.) We will return to this idea of using vectors when we discuss *valuation vectors* in Section 3, below.

At the conclusion of Section 3, we will introduce another exclusion criterion for Machin-type BBP arctangent formulae to show that any Machin-type BBP arctangent formula for π must be a binary formula. In particular, there is no decimal Machin-type BBP arctangent formula for π . This result is based on a technique which is also useful for excluding Machin-type BBP “logarithm formulae”—the topic to which we now turn.

3. MACHIN-TYPE BBP FORMULAE FOR LOGARITHMS

3.1. Machin-type logarithmic generators and formulae. Our definition of a Machin-type BBP logarithm formula is analogous to our definition of a Machin-type BBP arctangent formula, with $\Re \ln(z) = \ln |z|$ replacing the role of $\Im \ln(z)$. Although group theory plays a less important role here, we note that we are working with the multiplicative group $\mathbb{C}^\times/\mathbb{S}$. The group $\mathbb{C}^\times/\mathbb{S}$ is isomorphic to the additive group \mathbb{R} , under the isomorphism that sends $t \in \mathbb{R}$ to the coset $e^t\mathbb{S}$. The inverse map is $z\mathbb{S} \mapsto \Re \ln(z) = \ln |z|$. However, since $\mathbb{C}^\times/\mathbb{S}$ is so readily identified with the isomorphic multiplicative group \mathbb{R}_+^\times , we usually prefer to treat the latter group and its obvious isomorphism to the additive group \mathbb{R} , $\ln(z) : \mathbb{R}_+^\times \rightarrow \mathbb{R}$.

We begin by describing our *logarithmic generators*. (We give BBP formulae for these generators in Appendix A.) Given b not a proper power, $b > 2$, these are generators of the form $\ln(1 - b^{-m})$. In the case $b = 2$ we include additional *Aurifeuillian* generators, of the form $\ln |1 - (1 + i)2^{-m}|$. We call these additional generators Aurifeuillian because some terms which appear in the equation

$$\begin{aligned} \ln |1 \pm (1 + i)2^{-m}| &= \frac{1}{2} \ln (2^{1-2m}(2^{2m-1} \pm 2^m + 1)) \\ (43) \qquad \qquad \qquad &= \left(\frac{1}{2} - m\right) \ln(2) + \frac{1}{2} \ln(2^{2m-1} \pm 2^m + 1). \end{aligned}$$

correspond to factors in the equation due to Aurifeuille:

$$(44) \qquad 2^{4m-2} + 1 = (2^{2m-1} + 2^m + 1)(2^{2m-1} - 2^m + 1).$$

Definition 3. Given $\kappa \in \mathbb{R}$, $2 \leq b \in \mathbb{N}$, b not a proper power, we say that κ has a \mathbb{Z} -linear or \mathbb{Q} -linear *Machin-type BBP logarithm formula* to the base b if and only if κ can be written as a \mathbb{Z} -linear or \mathbb{Q} -linear combination (respectively) of generators of the form described in the previous paragraph. A non-Aurifeuillian formula is one which does not use Aurifeuillian generators. More briefly, when κ has a \mathbb{Q} -linear formula we will say that κ has a b -ary Machin-type BBP logarithm formula. ■

Remark. We call the generators of Definition 3 the *minimal set* of logarithm generators. From the identities $\ln(1 + b^{-m}) = \ln(1 - b^{-2m}) - \ln(1 - b^m)$

and $\ln|1 \pm ib^{-m}| = \ln(1 + b^{-2m})/2$ we find that our minimal set generates $\text{span}\{\ln(1 \pm b^{-m}), \ln|1 \pm ib^{-m}| : m \in \mathbb{N}\}$. The Aurifeuillian identity (44) implies that when $b = 2$ our minimal set generates

$$\text{span}\{\ln(1 \pm 2^{-m}), \ln|1 \pm i2^{-m}|, \ln|1 \pm (1 \pm i)2^{-m}| : m \in \mathbb{N}\}.$$

As in the arctangent case, for hand computations it is often convenient to use the “fuller set” of generators $\{\ln(1 \pm b^{-m}), \ln|1 \pm ib^{-m}|\}$, or the set

$$\{\ln(1 \pm 2^{-m}), \ln|1 \pm i2^{-m}|, \ln|1 \pm (1 \pm i)2^{-m}|\}$$

in the binary case. \square

3.2. Using valuation vectors and factorizations. When searching for Machin-type BBP logarithm formulae, we take much the same approach that we described for finding Machin-type BBP arctangent formulae for π . Given a finite set of generators of the form $\{\ln|z| : |z| \in \mathcal{G} \subset \mathbb{Q}[i]\}$, we begin by computing a *valuation vector* for each $|z|$, $|z| \in \mathcal{G}$. Let $\overline{\mathbb{Q}}$ denote the algebraic closure of \mathbb{Q} . (We allow $z \in \overline{\mathbb{Q}}$ so as to give a more general result, although we will only consider examples with $z \in \mathbb{Q}[i]$.) Given $z \in \overline{\mathbb{Q}}$, a valuation vector for z is a vector with entries indexed by a fixed set of primes \mathcal{P} , where the entry indexed by $p \in \mathcal{P}$ gives $\text{ord}_p(z)$. Note that $\text{ord}_p(z)$ can be extended so as to be defined for $z \in \overline{\mathbb{Q}}$ —see, for example, [Kob84, Chapter III]. For our purposes, it suffices to recall that $\text{ord}_p(zw) = \text{ord}_p(z) + \text{ord}_p(w)$, and thus $\text{ord}_p(1 - b^{-m}) = \text{ord}_p(b^m - 1) - m \text{ord}_p(b)$ while, as in the derivation of Equation (43), we find

$$\begin{aligned} \text{ord}_p(|1 - (1 + i)2^{-m}|) &= \text{ord}_p\left(2^{1/2-m} \sqrt{2^{2m-1} - 2^m + 1}\right) \\ (45) \qquad \qquad \qquad &= \left(\frac{1}{2} - m\right) \text{ord}_p(2) + \frac{1}{2} \text{ord}_p(2^{2m-1} - 2^m + 1). \end{aligned}$$

For example, indexing by the primes $\{2, 3, 5\}$ (in that order) the valuation vector for $1 - 2^{-4} = 15/16$ is $[-4, 1, 1]$, while the valuation vector for $|1 - (1 + i)2^{-4}| = \sqrt{2}\sqrt{113}/16$ is $[-3.5, 0, 0]$. In contrast, if we use $\mathcal{P} = \{2, 3, 5, 113\}$, the valuation vector for $|1 - (1 + i)2^{-4}|$ is $[-3.5, 0, 0, 1]$.

An important property of ord_p is that $|z| = \prod_p p^{\text{ord}_p(|z|)}$, where the product runs through all primes p for which $\text{ord}_p(|z|) \neq 0$. This implies that if we choose

$$\mathcal{P} = \bigcup_{|z| \in \mathcal{G}} \{p : \text{ord}_p(|z|) \neq 0\}.$$

then the vector space over \mathbb{Q} generated by $\{\ln|z| : |z| \in \mathcal{G}\}$ is isomorphic to the space of valuation vectors indexed by \mathcal{P} . Thus, in principle, it should be possible to reduce the task of searching for Machin-type BBP logarithm formulae (arising from a fixed set of generators) to doing \mathbb{Z} -linear algebra with valuation vectors, once again using the algorithms described in [Coh93, §2.4]. In practice, this might require finding the prime factorization of inordinately large numbers, in which case we can use a smaller set \mathcal{P} at the

cost of losing some information. Such a computational search is underway in our Centre.

Because of the nature of our generators, the task of finding Machin-type BBP formulae for logarithms is closely related to the *Cunningham Project* [BLS⁺88]: an ongoing project to find factorizations of numbers of the form $b^m \pm 1$, for $b \in \{2, 3, 5, 6, 7, 10, 11, 12\}$. As indicated above, one way to find the valuation vector for $1 - b^{-m}$ is to factor b and $b^m - 1$. Similarly, by Equation (45), we can find the valuation vector for $|1 - (1 + i)2^{-m}|$ by factoring b and $2^{2m-1} - 2^m + 1$. By the Aurifeuillian identity (44), the task of factoring $2^{2m-1} - 2^m + 1$ is closely related to the task of factoring $2^{4m-2} + 1$. One technique used in the Cunningham Project has been to break $b^m - 1$ into smaller factors by algebraically factoring $b^m - 1$ into cyclotomic polynomials $\psi_d(b)$, using the relationship

$$(46) \quad b^m - 1 = \prod_{d|m} \psi_d(b).$$

The cyclotomic polynomials can be defined by the inversion formula corresponding to (46), namely

$$(47) \quad \psi_d(b) = \prod_{m|d} (b^m - 1)^{\mu(d/m)},$$

where $\mu(d)$ denotes the Möbius function. (Cyclotomic polynomials are discussed in many references, for example [NZM91].)

In the case $b = 2$, the Aurifeuillian identity (44) is also useful as an algebraic factorization for $2^m - 1$. Further information about Aurifeuillian factorizations can be found in [Rie94, Appendix 6] and [Bre93]. A paper by Chamberland gives further discussion of the use of cyclotomic polynomials and Aurifeuillian factorizations to find BBP formulae [Cha].

3.3. Using Bang’s theorem as an exclusion criterion. Since formulae for $\ln(z)$, $z \in \mathbb{Q}$, can be generated as \mathbb{Z} -linear combinations of formulae for $\ln(p)$, p prime, most of the search for BBP formulae has focused on the latter case. However, as we will show below, Machin-type BBP formulae for $\ln(p)$ often fail to exist. Our main tool for excluding Machin-type BBP formulae for logarithms is a theorem due to Bang—which often goes under the name “Zsigmondy’s Theorem”, since Zsigmondy generalized Bang’s result. We will summarize Bang’s Theorem here, and present a more general discussion of Zsigmondy’s Theorem in Appendix C. We begin with a definition used in the statement of the theorem.

Definition 4. Given fixed $b > 1$, we will say that a prime p is a *primitive prime factor* of $b^m - 1$ if m is the least integer such that p divides $b^m - 1$. In other words, p is a primitive prime factor of $b^m - 1$ provided $\nu_b(p) = m$.

■

Theorem 3 (Bang, 1886). *The only cases where $b^m - 1$ has no primitive prime factor(s) are when $b = 2$, $m = 6$, $b^m - 1 = 3^2 \cdot 7$; and when $b = 2^N - 1$, $N \in \mathbb{N}$, $m = 2$, $b^m - 1 = 2^{N+1}(2^{N-1} - 1)$.*

We will call the cases where there is no primitive prime factor the “exceptional cases” of Bang’s Theorem, and will let M_b denote the value of m , depending on b , for which an exceptional case occurs, or $M_b := 0$ when there is no exceptional case. Thus

$$M_b := \begin{cases} 6 & \text{when } b = 2, \\ 2 & \text{when } b = 2^N - 1, N \in \mathbb{N}, \\ 0 & \text{otherwise.} \end{cases}$$

Bang’s Theorem can often be used to exclude the possibility of a constant having a Machin-type logarithm formula. We illustrate this with an example due to Carl Pomerance, first mentioned briefly in [BBP97, §5]:

Theorem 4. *There is no non-Aurifeuillian binary Machin-type BBP logarithms formula for $\ln(23)$ or for $\ln(89)$.*

Proof. Suppose instead that $\ln(23)$ has a non-Aurifeuillian binary Machin-type formula. This is equivalent to being able to write

$$(48) \quad 23^n = 2^t \prod_{m=1}^M (2^m - 1)^{n_m}$$

with $n_m \in \mathbb{Z}$, $n_M \neq 0$, $n \in \mathbb{N}$, and $t = -\sum_{m=1}^M m n_m$. Since $\nu_2(23) = 11$ we must have $M \geq 11$, so $2^M - 1$ has a primitive prime factor, say p . Since p cannot occur as a factor of $2^m - 1$, $m < M$, we must have $p = 23$, for otherwise we would not be able to cancel it out in (48). Since 23 is a primitive prime factor of $2^{11} - 1 = 23 \cdot 89$ we must have $M = 11$. But 89 is also a primitive prime factor $2^{11} - 1$, and cannot be canceled out of (48). The above argument also shows $\ln(89)$ can not be obtained. \blacksquare

The same argument applies of many other pairs of primes.

If we exclude Aurifeuillian generators, then to say $\ln(z)$ has a b -ary Machin-type BBP formula means $\ln(z) \in \text{span} \{\ln(1 - b^{-m}) : 1 \leq m \leq M\}$ for some $M < \infty$. A consequence of Bang’s Theorem is that, for fixed z , elements of the form $\ln(1 - b^{-m})$ and $\ln(z)$ have a strong tendency to be linearly independent, which excludes the possibility of a Machin-type BBP formula.

We now develop somewhat more technical tools for demonstrating linear independence of logarithms. Lemma 5 below gives a general criterion for linear independence for elements of the form $\ln(z)$, $z \in \overline{\mathbb{Q}}$. The idea behind Lemma 5 is to find a sequence of valuation vectors, which, when arranged in a matrix, give a triangular matrix with nonzero entries along the diagonal.

Lemma 5. *Given z_0, z_1, \dots, z_K , all elements of $\overline{\mathbb{Q}}$, then a sufficient condition that $\ln(z_0), \dots, \ln(z_K)$ be \mathbb{Q} -linearly independent is that there be*

distinct primes p_0, \dots, p_K with $\text{ord}_{p_k}(z_k) \neq 0$ and $\text{ord}_{p_j}(z_k) = 0$ when $j > k$.

Proof. If there were a \mathbb{Q} -linear dependence among the $\ln(z_k)$ then for some $n_k \in \mathbb{Z}$, not all zero, we would have

$$(49) \quad \sum_{k=0}^m n_k \ln(z_k) = 0, \quad \text{and so}$$

$$\prod_{k=0}^m z_k^{n_k} = 1,$$

where m denotes the largest k for which $n_k \neq 0$. Writing $n := n_m$ and $p := p_m$, our conditions give $\text{ord}_p(z_k) \neq 0$ if and only if $k = m$, while Equation (49) gives the contradiction

$$\text{ord}_p \left(\prod_{k=0}^m z_k^{n_k} \right) = n \text{ord}_p(z_m) = 0.$$

■

Theorem 6, below, gives a fairly general exclusion criterion for Machin-type BBP logarithm formulae. In our proof we will make use of the fact that if $\text{ord}_p(b^m - 1) \neq 0$ then $\text{ord}_p(b) = 0$ and, furthermore, $\text{ord}_p(1 - b^{-k}) = \text{ord}_p(b^k - 1)$, for any $k \in \mathbb{Z}$.

Theorem 6. *Given $z_0 \in \overline{\mathbb{Q}}$ and $2 \leq b \in \mathbb{N}$, b not a proper power, assume that there is at least one prime p such that $\text{ord}_p(z_0) \neq 0$ (equivalently, assume that z_0 is not a root of unity) and let p_0 be the largest such prime. Let*

$$(50) \quad M_0 := \max(M_b, p_0 - 1),$$

with M_b given below Theorem 3, and let

$$U := \text{span} \{ \ln(1 - b^{-m}) : 1 \leq m \leq M_0 \}.$$

Note that U has a basis of the form $\ln(z_k)$, $1 \leq k \leq \dim(U)$. If there are distinct primes $p_1, \dots, p_{\dim(U)}$ such that for $0 \leq j, k \leq \dim(U)$ we have $\text{ord}_{p_k}(z_k) \neq 0$ and $\text{ord}_{p_j}(z_k) = 0$ when $j > k$, then there is no non-Aurifeuillian \mathbb{Q} -linear Machin-type BBP logarithm formula for $\ln(z_0)$.

Proof. Suppose, to the contrary, that there is a Machin-type BBP formula for $\ln(z_0)$, i.e., $\ln(z_0) \in V := \text{span} \{ \ln(1 - b^{-m}) : 1 \leq m \leq M \}$ for some $M < \infty$. Without loss of generality, we may assume $M \geq M_0$, i.e., $U \subseteq V$. For $k > \dim(U)$ let $m_k := M_0 + k - \dim(U)$, so m_k ranges over $M_0 + 1 \leq m_k \leq M$ as k ranges over $\dim(U) + 1 \leq k \leq \dim(U) + M - M_0$. Let $z_k := 1 - b^{-m_k}$, and let p_k denote a primitive prime factor of $b^{m_k} - 1$. (Note that p_k exists since $m_k > M_0 \geq M_b$.) Clearly, $V = \text{span} \{ \ln(z_k) : 0 \leq k \leq \dim(U) + M - M_0 \}$. We will show that z_k, p_k , $0 \leq k \leq \dim(U) + M - M_0$ satisfy the conditions of Lemma 5. This will

establish our result since the linear independence of $\ln(z_k)$ contradicts our assumption that $\ln(z_0) \in V$.

To show that our z_k, p_k satisfy the conditions of Lemma 5 we first note that $\text{ord}_{p_k}(z_k) \neq 0$ by our assumptions and the fact that, for $k > \dim(U)$, we have $\text{ord}_{p_k}(1 - b^{-m_k}) = \text{ord}_{p_k}(b^{m_k} - 1) \neq 0$. It remains to show that $\text{ord}_{p_j}(z_k) = 0$ when $j > k$.

We first treat the case $k = 0$. By assumption, $\text{ord}_{p_j}(z_0) = 0$ for $1 \leq j \leq \dim(U)$. For $j > \dim(U)$, p_j is a primitive prime factor of $b^{m_j} - 1$, and $m_j > M_0$. By Fermat's "Little Theorem", we know that if p is a primitive prime factor of $b^m - 1$ then $m \mid p - 1$ and thus $p \geq m + 1$. Thus $p_j \geq m_j + 1 > M_0 + 1 \geq p_0$, and it follows that $\text{ord}_{p_j}(z_0) = 0$ since, by definition, p_0 is the largest prime such that $\text{ord}_{p_0}(z_0) \neq 0$.

We next treat the case $1 \leq k \leq \dim(U)$. Again, by assumption, $\text{ord}_{p_j}(z_k) = 0$ for $1 \leq k < j \leq \dim(U)$. Since $\ln(z_k) \in U$, we know that $\ln(z_k)$ is a \mathbb{Q} -linear combination of elements of the form $\ln(1 - b^{-m})$, $1 \leq m \leq M_0$. Thus, there are $n_m \in \mathbb{Z}$, not all zero, and some $n \neq 0$, such that

$$(51) \quad z_k^n = \prod_{m=1}^{M_0} (1 - b^{-m})^{n_m}.$$

Now, when $j > \dim(U)$ we have $\text{ord}_{p_j}(1 - b^{-m}) = 0$ for $1 \leq m \leq M_0$, since p_j is a primitive prime factor of $b^{m_j} - 1$ and $m_j > M_0$. From this and Equation (51) it follows that

$$\text{ord}_{p_j}(z_k) = \frac{1}{n} \sum_{m=1}^{M_0} n_m \text{ord}_{p_j}(1 - b^{-m}) = 0.$$

Finally, when $\dim(U) < k < j$, $\text{ord}_{p_j}(z_k) = 0$ follows from the fact that p_j is a primitive prime factor of $b^{m_j} - 1$. \blacksquare

Remark. Theorem 6 implies that when searching for a non-Aurifeuillian Machin-type BBP logarithm formula for $\ln(z_0)$, one only need consider the generators $\ln(1 - b^{-m})$, $1 \leq m \leq M_0$, where M_0 is defined by Equation (50). \square

Example 4. When $M_b = 0$ it follows that there is no Machin-type BBP logarithm formula for $\ln(b)$ to the base b . In particular, there is no decimal Machin-type BBP logarithm formula for $\ln(10)$. Here we use $z_0 = b$, p_0 the largest prime divisor of b . For $k > 0$ we use $z_k := 1 - b^{-k}$ and choose p_k to be any primitive prime factor of $b^k - 1$, noting that p_k exists since $M_b = 0$. Our result then follows immediately from Theorem 6. Since, when $M_b = 0$, there is no b -ary formula for $\ln(b)$, it seems somewhat unlikely in this case that there is a b -ary formula for any $\ln(n)$, $n \in \mathbb{N}$, but we have been unable to prove this. \square

Example 5. When $b = 7 = 2^3 - 1$ we have $M_b = 2$, and the argument of the previous example does not apply. However, again we find that there is no 7-ary Machin-type BBP logarithm formula for $\ln(7)$. Here we have $z_0 = 7$,

$p_0 = 7$. Since $M_0 = \max(M_b, p_0 - 1) = 6$, we need to find suitable z_k, p_k for $1 \leq k \leq 6$. We begin with $z_1 = 8/7, p_1 = 2; z_2 = 48/49 = 1 - 7^{-2}, p_2 = 3$. For $k > M_b = 2$ we can simply use $z_k = 1 - 7^{-k}, p_k$ some primitive prime factor of $7^k - 1$. We can easily see that the conditions for Theorem 6 are satisfied, and the result follows. \square

Remark. In Example 5, when $k = 1$ we had to modify the “obvious” choice of basis element, namely $z_k = 1 - 7^{-k}$, in order to make our p_k satisfy the conditions of Theorem 6. In particular, we require $\text{ord}_3(z_1) = 0$. We accomplished this task by using valuation vectors. Here, indexing by the primes $\{7, 2, 3\}$ (in that order), the valuation vector for 7 is $v_0 := [1, 0, 0]$, while the vectors for $1 - 7^{-1} = 6/7$ and $1 - 7^{-2} = 48/49$ are $v_1 := [-1, 1, 1]$ and $v_2 := [-2, 4, 1]$ respectively. Searching for z_1 such that $\text{ord}_3(z_1) = 0$ lead us to find the valuation vector $[-1, 3, 0] = v_2 - v_1$, and thus $z_1 = 7^{-1} \cdot 2^3 = 8/7$. \square

Example 6. To demonstrate the result of Theorem 4 in the language of Theorem 6, we begin with $z_0 = 23, p_0 = 23, z_1 = 1 - 1/2, p_1 = 2$. Our rule of thumb starting with $k = 2$ will be to use $z_k = 1 - 2^{-m_k}$ for an increasing sequence m_k , and to choose p_k to be a primitive prime factor of $2^{m_k} - 1$. Thus, $z_2 = 1 - 2^{-2} = 3/4, p_2 = 3, z_3 = 1 - 2^{-3} = 7/8, p_3 = 7, \dots$ We let $m_6 = 7$ rather than 6, since $\ln(1 - 2^{-6})$ is linearly dependent on earlier $\ln(z_k)$. Continuing in this manner, letting $m_{k+1} = m_k + 1$, we come to $z_{10} = 1 - 2^{-11}$. We have $2^{11} - 1 = 23 \cdot 89$, both factors being primitive prime factors. Since $23 = p_0$, we choose $p_{10} = 89$. For $k > 10$ we may continue using our rule of thumb, with no complications, through $m_k = M_0 = 22$, at which point we have established the necessary conditions for Theorem 6.

As in previous examples, we see that it is not always necessary to present p_k explicitly. More specifically, when $m_k > M_b$ we are assured that $b^{m_k} - 1$ has a primitive prime factor p_k , and to guarantee that p_k has not occurred earlier in our sequence we only need check that $\gcd(z_0, b^{m_k} - 1) = 1$. \square

Remarks. i.) We have been unable to exclude the possibility that there might be a binary Machin-type BBP logarithm formula for $\ln(23)$ that uses some Aurifeuillian generators, although it seems unlikely. Using Equation (45), and some simple number theory, one can also show for odd primes p that $\text{ord}_p(|1 - (1 + i)2^{-m}|) \neq 0$ implies $\nu_2(p) \equiv 0 \pmod{4}$. This restricts the possibilities for any Aurifeuillian binary Machin-type BBP logarithm formula for $\ln(23)$ and suggests that any such representation must have truly “massive” generators, if it exists at all.

ii.) The next two primes with logarithms for which no binary formula has been found are 47 and 53. Again, in each case the prime shares a prime friend which is also a primitive prime factor of the same $2^M - 1$. We have $2^{23} - 1 = 47 \cdot 178481$, and $\nu_2(178481) = \nu_2(47) = 23$. Also since 4 has order 23 mod 178481, the factor 178481 (as with 47) does not occur in the other Aurifeuillian factors. Thus, $\ln(1 - 2^{-1081m})$ or some larger terms must be

used. For example, $2^{1081} - 1$ has two factors of order 1081 and many other terms would be needed to split them!

Likewise $\nu_2(53) = 52$ and $2^{52} - 1 = 15 \cdot \mathbf{53} \cdot \mathbf{157} \cdot \mathbf{1613} \cdot 2731 \cdot 8191$ where $\nu_2(p) = 52$ for each bold factor p . In this last case however $2^{2n-1} \pm 2^{n+1} + 1$ can also be a multiple of 53, since the order of 4 is not odd.

iii.) It is interesting to contrast $\ln(23)$ with $\ln(113)$, since the cases are similar, but $\ln(113)$ *does* have an Aurifeuillian binary Machin-type BBP logarithm formula. Here we have $\nu_2(113) = 28$, and $2^{28} - 1 = 3 \cdot 5 \cdot 29 \cdot 43 \cdot 113 \cdot 127$. Since we also have $\nu_2(29) = 28$, the argument of Theorem 4 can be adapted to show that $\ln(113)$ has no non-Aurifeuillian binary Machin-type BBP logarithm formula. However, using Equation (44), we find that

$$2^{28} - 1 = (2^{14} - 1)(2^7 + 2^4 + 1)(2^7 - 2^4 + 1),$$

where $2^7 - 2^4 + 1 = 113$. Using Equation (43), it follows that

$$\ln(113) = 2 \ln |1 - (1 + i)2^{-4}| - 7 \ln(1 - 2^{-1}),$$

which is a linear combination of binary Machin-type logarithmic generators. \square

3.4. An application to arctangent formulae. We conclude this section by applying Theorem 3 (Bang's Theorem) to demonstrate that there are no b -ary Machin-type *arctangent formulae* for π unless $b = 2$.

Theorem 7. *Given $b > 2$ and not a proper power, there is no \mathbb{Q} -linear b -ary Machin-type BBP arctangent formula for π .*

Proof. It follows immediately from the definition of a \mathbb{Q} -linear Machin-type BBP arctangent formula (Definition 1) that any such formula has the form

$$(52) \quad \pi = \frac{1}{n} \sum_{m=1}^M n_m \mathfrak{S} \ln(b^m - i),$$

where $n \in \mathbb{N}$, $n_m \in \mathbb{Z}$, and $M \geq 1$, $n_M \neq 0$. This implies that

$$(53) \quad \prod_{m=1}^M (b^m - i)^{n_m} \in e^{ni\pi} \mathbb{Q}^\times = \mathbb{Q}^\times.$$

For any $b > 2$ and not a proper power we have $M_b \leq 2$, so it follows from Bang's Theorem that $b^{4M} - 1$ has a primitive prime factor, say p . Furthermore, p must be odd, since $p = 2$ can only be a *primitive* prime factor of $b^m - 1$ when b is odd and $m = 1$. Since p is a primitive prime factor, it does not divide $b^{2M} - 1$, and so p must divide $b^{2M} + 1 = (b^M + i)(b^M - i)$. We cannot have both $p \mid b^M + i$ and $p \mid b^M - i$, since this would give the contradiction that $p \mid (b^M + i) - (b^M - i) = 2i$. It follows that $p \equiv 1 \pmod{4}$, and that p factors as $p = \mathfrak{p}\bar{\mathfrak{p}}$ over $Z[i]$, with exactly one of \mathfrak{p} , $\bar{\mathfrak{p}}$ dividing $b^M - i$. Referring to Definition 2, we see that we must have $\vartheta_p(b^M - i) \neq 0$. Furthermore, for any $m < M$ neither \mathfrak{p} nor $\bar{\mathfrak{p}}$ can divide $b^m - i$ since this would imply $p \mid b^{4m} - 1$, $4m < 4M$, contradicting the

fact that p is a primitive prime factor of $b^{4M} - 1$. So for $m < M$ we have $\vartheta_p(b^m - i) = 0$. Referring to Equation (53), using Equation (41) and $n_M \neq 0$, we get the contradiction that

$$0 \neq n_M \vartheta_p(b^M - i) = \sum_{m=1}^M n_m \vartheta_p(b^m - i) = \vartheta_p(\mathbb{Q}^\times) = 0.$$

Thus, our assumption that there was a b -ary Machin-type BBP formula for π must be false. \blacksquare

We finish the section with our deferred proof.

Proof of Theorem 2b.

Proof. It again follows from the definition of a \mathbb{Q} -linear Machin-type BBP arctangent formula (Definition 1) that any such formula has the form

$$(54) \quad \arctan(y/x) = \Im \ln(x + iy) = \frac{1}{n} \sum_{m=1}^M n_m \Im \ln(b^m - i),$$

where $n \in \mathbb{N}$, $n_m \in \mathbb{Z}$, and $M \geq 1$, $n_M \neq 0$. This implies that

$$(55) \quad \prod_{m=1}^M (b^m - i)^{n_m} \in (x + iy)^n \mathbb{Q}^\times.$$

It follows from Bang's Theorem that $b^{4M} - 1$ has a primitive prime factor, say p' . Furthermore, p' must be odd, since $p' = 2$ can only be a *primitive* prime factor of $b^m - 1$ when b is odd and $m = 1$. Since p' is a primitive prime factor, it does not divide $b^{2M} - 1$, and so p' must divide $b^{2M} + 1 = (b^M + i)(b^M - i)$. Again, we cannot have both $p' \mid b^M + i$ and $p' \mid b^M - i$, since this would give the contradiction that $p' \mid (b^M + i) - (b^M - i) = 2i$. It follows that $p' \equiv 1 \pmod{4}$, and that p' factors as $p' = \mathfrak{p}' \overline{\mathfrak{p}'}$ over $Z[i]$, with exactly one of \mathfrak{p}' , $\overline{\mathfrak{p}'}$ dividing $b^M - i$.

Hence, referring to Equation (55), using Equation (41) and $n_M \neq 0$, we get that

$$0 \neq n_M \vartheta_{p'}(b^M - i) = \sum_{m=1}^M n_m \vartheta_{p'}(b^m - i) = \vartheta_{p'}(x + iy)^n.$$

In consequence $p' = p$, since p is the unique prime divisor of $x^2 + y^2$ congruent to 1 modulo 4. It follows that $4M = \nu_b(p) = \nu_b(q)$ and hence, much as above, that

$$0 \neq n_M \vartheta_q(b^M - i) = \sum_{m=1}^M n_m \vartheta_q(b^m - i) = \vartheta_q(x + iy)^n = 0,$$

where the final equality is by hypothesis. Thus, our assumption that there was a non-Aurifeuillian b -ary Machin-type BBP formula for $\arctan(x/y)$ must be false. \blacksquare

4. ACKNOWLEDGMENTS

Carl Pomerance was the first to observe the importance of Bang’s theorem as a tool for excluding the possibility of non-Aurifeuillian logarithm formulae. Pomerance also provided references for some of the papers, cited below, that generalize Zsigmondy’s Theorem. Imin Chen and Nils Bruin gave advice on various aspects of ord_p and algebraic number theory. The material in Appendix B is adapted from notes provided by David Bailey.

APPENDIX A. BBP FORMULAE FOR MACHIN-TYPE BBP GENERATORS

For b not a proper power, $b > 2$ our arctangent generators are

$$\arctan(-b^{-m}) = \Im \ln(1 - ib^{-m}) = b^{-3m} P(1, b^{4m}, 4, [-b^{2m}, 0, 1, 0]).$$

When $b = 2$, we also use the “Aurifeuillian” generators

$$\begin{aligned} \arctan(1/(1 - 2^m)) &= \Im \ln(1 - (1 + i)2^{-m}) \\ &= 2^{-7m+3} P(1, 2^{8m-4}, 8, [-2^{6m-3}, -2^{5m-2}, -2^{4m-2}, 0, 2^{2m-1}, 2^m, 1, 0]). \end{aligned}$$

For b not a proper power, $b > 2$ our logarithmic generators are

$$\ln(1 - b^{-m}) = -b^{-m} \sum_{k \geq 0} \frac{1}{k+1} b^{-mk}.$$

In terms of Bailey’s $P(s, b, n, A)$, these generators are

$$\ln(1 - b^{-m}) = -b^{-m} P(1, b^m, 1, [1]).$$

When $b = 2$, we also use the “Aurifeuillian” generators

$$\begin{aligned} \ln |1 - (1 + i)2^{-m}| \\ = 2^{-8m+4} P(1, 2^{8m-4}, 8, [-2^{7m-4}, 0, 2^{5m-3}, 2^{4m-2}, 2^{3m-2}, 0, -2^{m-1}, -1]). \end{aligned}$$

The BBP formulae for both the arctangent and logarithmic Aurifeuillian generators may be derived by extracting imaginary and real parts (for arctangent and logarithmic generators, respectively) from the formula

$$\begin{aligned} \ln(1 - (1 + i)2^{-m}) &= - \sum_{r=1}^8 2^{-mr} (1 + i)^r \sum_{k \geq 0} \frac{(1 + i)^{8k}}{8k + r} 2^{-8mk} \\ &= - \sum_{r=1}^8 2^{-mr} (1 + i)^r \sum_{k \geq 0} \frac{1}{8k + r} 2^{(4-8m)k}. \end{aligned}$$

APPENDIX B. CONVERSION TO POLYLOGARITHMIC FORMULAE

In this Appendix we will analyze vector spaces of constants with *polylogarithmic* BBP formulae, i.e., constants κ which have the form

$$(56) \quad \kappa = \sum_{k \geq 0} \sum_{j=1}^n \frac{a_j}{(nk + j)^s} b^{-mk} = P(s, b^m, n, [a_1, \dots, a_n]),$$

with $a_j \in \mathbb{Q}$, $s, b, m, n \in \mathbb{N}$, $b > 1$. Our main purpose is to demonstrate that any constant with a Machin-type BBP formula also has a polylogarithmic BBP formula. (Although our interest will be focused on the case where b is not a proper power we allow any $b \in \mathbb{N}$, $b > 1$.)

Definition 5. Recall that $\text{span}\{\alpha_k\}$ denotes the vector space over \mathbb{Q} spanned by the set $\{\alpha_k\}$. Given $s, b, m, n \in \mathbb{N}$, $b > 1$, let

$$\begin{aligned} V_{s,b,m,n} &:= \text{span} \left\{ \sum_{k \geq 0} \frac{1}{(nk+j)^s} b^{-mk} : 1 \leq j \leq n \right\}, \\ V_{s,b,m} &:= \text{span} \left\{ \bigcup_{n \geq 1} V_{s,b,m,n} \right\}, \\ V_{s,b} &:= \text{span} \left\{ \bigcup_{m \geq 1} V_{s,b,m} \right\}. \end{aligned}$$

■

Referring to Appendix A, we see that our non-Aurifeuillian arctangent generators, $\arctan(-b^{-m})$, lie in $V_{1,b,4m,4}$. The Aurifeuillian arctangent generators, $\arctan(1/(1-2^m))$, lie in $V_{1,2,8m-4,8}$. In the case of our logarithmic generators we have $\ln(1-b^{-m}) \in V_{1,b,m,1}$ (non-Aurifeuillian generators), while $\ln|1-(1+i)2^{-m}| \in V_{1,2,8m-4,8}$ (Aurifeuillian generators).

Lemma 8. *Given $d \in \mathbb{N}$ we have*

$$(57) \quad V_{s,b,m,n} \subseteq V_{s,b,m,dn},$$

and

$$(58) \quad V_{s,b,m} \subseteq V_{s,b,dm,dn}.$$

Proof. To establish (57) we note that $\kappa \in V_{s,b,m,n}$ is equivalent to

$$\begin{aligned} (59) \quad \kappa &= \sum_{j=1}^n \sum_{k \geq 0} \frac{a_j}{(nk+j)^s} b^{-mk} \\ &= \sum_{j=1}^n \sum_{k \geq 0} \frac{d^s a_j}{(dnk+dj)^s} b^{-mk} \\ &= \sum_{j=1}^{dn} \sum_{k \geq 0} \frac{a'_j}{(dnk+j)^s} b^{-mk} \in V_{s,b,m,dn}; \end{aligned}$$

where we let

$$a'_j := \begin{cases} d^s a_{j/d} & \text{when } d \mid j, \\ 0 & \text{otherwise.} \end{cases}$$

Similarly, to establish (58) we proceed from Equation (59) to find

$$\begin{aligned}\kappa &= \sum_{j=1}^n \sum_{k \geq 0} \sum_{r=0}^{d-1} \frac{a_j b^{-mr}}{(dnk + nr + j)^s} b^{-dmk} \\ &= \sum_{j'=1}^{dn} \sum_{k \geq 0} \frac{a'_{j'}}{(dnk + j')^s} b^{-dmk} \in V_{s,b,dm,dn};\end{aligned}$$

where we let $j' := nr + j$, so that $r = \lfloor j'/n \rfloor$, $j \equiv j' \pmod{n}$, $1 \leq j \leq n$, and where $a'_{j'} := a_j b^{-mr}$. \blacksquare

Theorem 9. *Given $\kappa \in V_{s,b,m}$ then $\kappa \in V_{s,b,m,n}$, where n depends on κ .*

Proof. Let $\kappa = \kappa_1 + \kappa_2$ where $\kappa_1 \in V_{s,b,m,n_1}$, $\kappa_2 \in V_{s,b,m,n_2}$. From (57), it follows that both κ_1 and κ_2 are elements of $V_{s,b,m,\text{lcm}(n_1,n_2)}$, and thus $\kappa \in V_{s,b,m,\text{lcm}(n_1,n_2)}$.

By definition, $\kappa \in V_{s,b,m}$ means that

$$(60) \quad \kappa = \sum_q \alpha_q \kappa_q,$$

where $\alpha_q \in \mathbb{Q}$, $\kappa_q \in V_{s,b,m,n_q}$, and where the sum is finite. By using induction on the number of terms on the right side of (60), applying the result of the previous paragraph when summing two terms, the conclusion follows. \blacksquare

Theorem 10. *Given $\kappa \in V_{s,b}$ then $\kappa \in V_{s,b,m,n}$, where m, n depend on κ .*

Proof. Let $\kappa = \kappa_1 + \kappa_2$ where $\kappa_1 \in V_{s,b,m_1}$, $\kappa_2 \in V_{s,b,m_2}$. By Theorem 9 we may assume that $\kappa_1 \in V_{s,b,m_1,n_1}$, $\kappa_2 \in V_{s,b,m_2,n_2}$. Applying (58) and then (57), it follows that both κ_1 and κ_2 are elements of $V_{s,b,\text{lcm}(m_1,m_2),\text{lcm}(N_1,N_2)}$, where $N_1 := n_1 m_2 / \gcd(m_1, m_2)$, $N_2 := n_2 m_1 / \gcd(m_1, m_2)$.

By definition $\kappa \in V_{s,b}$ means that

$$(61) \quad \kappa = \sum_q \alpha_q \kappa_q,$$

where $\alpha_q \in \mathbb{Q}$, $\kappa_q \in V_{s,b,m_q}$, and where the sum is finite. By using induction on the number of terms on the right side of (61), applying the result of the previous paragraph when summing two terms, the conclusion follows. \blacksquare

The above proofs implicitly give a constructive method for finding a polylogarithmic BBP formula for any element of $V_{s,b}$. In particular we may find a polylogarithmic BBP formula for any constant with a b -ary Machin-type BBP formulae, since such constants lie within $V_{1,b}$. For example, in Section 2.5 we found that $\arctan(1/6) = \arctan(1/5) - \arctan(1/31)$.

Referring to Appendix A, and using Bailey's $P(s, b, n, A)$, we have

$$\begin{aligned}\arctan(1/5) &= 2^{-11} P(1, 2^{12}, 8, [2^9, -2^8, 2^6, 0, -2^3, 2^2, -1, 0]) \in V_{1,2,12,8}, \\ \arctan(1/31) &= 2^{-32} P(1, 2^{36}, 8, [2^{27}, 2^{23}, 2^{18}, 0, -2^9, -2^5, -1, 0]) \in V_{1,2,36,8}.\end{aligned}$$

Note that Appendix A covers $\arctan(1/5)$ as it equals $\arctan(1/3) - \arctan(1/8)$, by the note at the end of section 2.4. Applying (58) from Lemma 8, we can re-express $\arctan(1/5)$ as an element of $V_{1,2,36,24}$, giving

$$\begin{aligned} \arctan(1/5) = 2^{-11} P(1, 2^{36}, 24, [2^9, -2^8, 2^6, 0, -2^3, 2^2, -1, 0, \\ 2^{-3}, -2^{-4}, 2^{-6}, 0, -2^{-9}, 2^{-10}, -2^{-12}, 0, \\ 2^{-15}, -2^{-16}, 2^{-18}, 0, -2^{-21}, 2^{-22}, -2^{-24}, 0]). \end{aligned}$$

We then apply (57) in order to re-express $\arctan(1/31)$ as an element of $V_{1,2,36,24}$, giving

$$\begin{aligned} \arctan(1/31) = 2^{-32} P(1, 2^{36}, 24, \\ [0, 0, 3 \cdot 2^{27}, 0, 0, 3 \cdot 2^{23}, 0, 0, 3 \cdot 2^{18}, 0, 0, 0, \\ 0, 0, -3 \cdot 2^9, 0, 0, -3 \cdot 2^5, 0, 0, -3, 0, 0, 0]). \end{aligned}$$

Finally, taking the difference of these two results and factoring out the denominator from the vector of coefficients, we get

$$\begin{aligned} \arctan(1/6) &= \arctan(1/5) - \arctan(1/31) \\ &= 2^{-35} P(1, 2^{36}, 24, \\ &\quad [2^{33}, -2^{32}, -2^{31}, 0, -2^{27}, -2^{27}, -2^{24}, 0, \\ &\quad -2^{22}, -2^{20}, 2^{18}, 0, -2^{15}, 2^{14}, 2^{13}, 0, \\ &\quad 2^9, 2^9, 2^6, 0, 2^4, 2^2, -1, 0]). \end{aligned}$$

APPENDIX C. ZSIGMONDY'S THEOREM

This summary of Zsigmondy's theorem and related results is paraphrased, almost verbatim, from Paulo Ribenboim's *The Little Book of BIG Primes* [Rib91].

Given natural numbers a, b , we say that a prime p is a primitive prime factor of $b^m - a^m$ if m is the least integer such that p divides $b^m - a^m$ (resp., $b^m + a^m$, when studying that case; $b^m \pm a^m$ are both of interest).

Theorem 11 (K. Zsigmondy, 1892).

If $b > a \geq 1$ and $\gcd(a, b) = 1$ then every number $b^m - a^m$ has a primitive prime factor—the only exceptions being $a = 1, b = 2, m = 6$ and $a + b = \text{power of two}$ (thus, a, b odd), $m = 2$.

Equally, every number $b^m + a^m$ has a primitive prime factor—with the exception of $2^3 + 1 = 9$.

The special case where $a = 1$ had been proved by Bang in 1886. Later proofs were given by Birkhoff and Vandiver (1904), Carmichael (1913), Kanold (1950), Artin (1955), Lüneburg [Lün81], “and probably others”.

Define t_m^* to be the “primitive part” of $b^m - a^m$, i.e. $b^m - a^m = t_m^* t'_m$ with $\gcd(t_m^*, t'_m) = 1$ and where $p \mid t_m^*$ if and only if p is a primitive prime factor of $b^m - a^m$. Numerical experience shows that t_m^* is composite apart from a few initial values.

Let $k(n)$ denote the “square-free kernel” of n , i.e., n divided by its largest square factor, and let $e = 1$ if $k(ab) \equiv 1 \pmod{4}$, $e = 2$ if $k(ab) \equiv 2, 3 \pmod{4}$. Schinzel has shown [Sch62] that if $m/(ek(ab))$ is an odd integer then $b^m - a^m$ has at least two distinct primitive prime factors, with the following exceptions when $m > 1$:

$$a = 1, b = 2, m \in \{4, 12, 20\};$$

$$a = 1, b = 3, m = 6;$$

$$a = 2, b = 3, m = 12;$$

$$a = 1, b = 4, m = 3;$$

$$a = 3, b = 4, m = 6.$$

Schinzel also proved that if $ab = c^h$ for $h \geq 3$, then there are infinitely many m such that the primitive part of $b^m - a^m$ has at least three prime factors.

APPENDIX D. DENSITY RESULTS

In this appendix we will discuss various results on the density of arctangents which have Machin-type BBP arctangent formulae. We begin by noting that if $\theta = \arctan(\rho)$ has a Machin-type BBP formula then any element of $\theta\mathbb{Q}$ has a \mathbb{Q} -linear arctangent formula. For a fixed base b , we have Machin-type BBP arctangent formulae for $\Im \ln(1 - ib^{-m})$, so any one of these will generate a dense set of $\theta \in \mathbb{R}$ with base b \mathbb{Q} -linear Machin-type BBP arctangent formula. If, in order to be considered an “arctangent”, we prefer the convention that θ satisfies $-\pi/2 < \theta < \pi/2$, it remains clear that the set of $\theta \in (-\pi/2, \pi/2)$ with a \mathbb{Q} -linear Machin-type BBP arctangent formula is dense.

If we prefer to restrict ourselves to θ with \mathbb{Z} -linear arctangent formulae, then the set $n\theta$, $n \in \mathbb{Z}$, is not dense in \mathbb{R} . On the other hand, if we write $\theta = \Im \ln(x+iy)$ and define x_n, y_n to satisfy $x_n + iy_n := (x+iy)^n$, $n \in \mathbb{Z}$, then $n\theta \equiv \Im \ln(x_n + iy_n) \equiv \arctan(y_n/x_n) \pmod{\pi}$. In other words $\tan(n\theta) = y_n/x_n$ for all $n \in \mathbb{Z}$. By [NZM91, Theorem 6.16], θ cannot be a rational multiple of π unless $\tan(\theta) \in \{0, \pm 1, \infty\}$. In particular, for fixed $b \geq 2$, $\theta = \Im \ln(1 - ib^{-m}) = \arctan(-b^{-m})$ is not a rational multiple of π for any $m \in \mathbb{N}$, since $-b^{-m} \notin \{0, \pm 1, \infty\}$. It follows by Weyl’s theorem [HW79, Theorem 445] that for such θ the sequence $n\theta$ is uniformly distributed modulo π . Thus, if there is a b -ary \mathbb{Z} -linear Machin-type BBP formula for π then the set $n_1\theta + n_2\pi$, $n_1, n_2 \in \mathbb{Z}$, is dense in the interval $(-\pi/2, \pi/2)$, and clearly $n_1\theta + n_2\pi$ has a b -ary \mathbb{Z} -linear Machin-type BBP arctangent formula. If there is no b -ary \mathbb{Z} -linear Machin-type BBP formula for π then we may still conclude that $\{\tan(n\theta) : n \in \mathbb{Z}\}$ is dense in \mathbb{R} .

Finally, suppose that b and $x + iy$ satisfy the conditions of Theorem 2. That is, suppose there is a prime $p \nmid b$, $p \equiv 1 \pmod{4}$, $4 \nmid \nu_b(p)$, and $\vartheta_p(x + iy) \neq 0$. By Theorem 2, there is no \mathbb{Q} -linear Machin-type BBP

formula for $\arctan(y/x)$. Furthermore, since $\vartheta_p((x + iy)^n) = n\vartheta_p(x + iy)$, there is no \mathbb{Q} -linear Machin-type BBP formula for $\arctan(y_n/x_n)$ for any $n \neq 0$, $n \in \mathbb{Z}$. Thus, provided $x/y \notin \{0, \pm 1, \infty\}$, the set $\{\arctan(y_n/x_n)\}$ is dense in \mathbb{R} , and no member of the set has a b -ary \mathbb{Q} -linear arctangent formula.

APPENDIX E. COMMENTS AND RESEARCH PROBLEMS

We've tried to arrange these comments in rough order of difficulty, ranging from nearly trivial to significant research topics.

- (1) Note that $3 + i = 2 + (1 + i) = 4 - (1 - i)$. This gives two distinct binary Machin-type BBP formulae for $\arctan(1/3)$. Should we count this as a trivial zero relation, or is it “interesting”?
- (2) How many \mathbb{Q} -linearly-independent binary Machin-type BBP arctangent zero relations can we find? Can we show that there is an upper bound on their number?
- (3) The first BBP formula found for π (presented in [BBP97]) was

$$(62) \quad \pi = \sum_{k \geq 0} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right) 2^{-4k}.$$

This formula does not appear to be a \mathbb{Q} -linear combination of Machin-type BBP generators. (Equation (63), below, can be used as an aid in seeing this.) Is there some simple way to derive (62) from a Machin-type BBP formula?

- (4) A consequence of Schinzel's result [Sch62], in the notation of Appendix C, is that if $b > 2$, $m > 12$, and $m/(e k(b))$ is odd, then $b^m - 1$ has at least two primitive prime factors. This implies that the logarithms of an infinity of primes have no b -ary Machin-type BBP logarithm formula, $b > 2$. One can work out the details, following the plan of Example 6.
- (5) If there are infinitely many primes $p \equiv 1 \pmod{4}$ for which $4 \nmid \nu_b(p)$, then by Theorem 2 this gives infinitely many examples base b with no b -ary Machin-type BBP arctangent formula. Does the existence of an infinity of such p follow from Chebotarëv's density theorem, or some other well-known result?
- (6) Our main tool has been group homomorphisms like $z \mapsto \text{ord}_p(z)$ and $z \mapsto \vartheta_p(z)$. When $\text{ord}_p(z) = 0$ can we make similar use of the homomorphism $z \mapsto (z/p)$ arising from the Jacobi symbol (z/p) ? Since $(z/p) \in \{-1, 1\}$ when $\text{ord}_p(z) = 0$, each such homomorphism would only give a “bit” of information. However, it should be possible to get more information by choosing many such p .
- (7) Our idea of using ord_p and ϑ_p works best when we can factor numbers rapidly. Since factorization is a difficult task in general, can we combine our approach with the use of an integer relation algorithm

such as PSLQ? The idea would be to find the “easy” factors, and use the resulting information to help guide PSLQ.

- (8) Zsigmondy’s theorem has been generalized to number fields [Sch74]. (See also [BHV01], which Carl Pomerance has described as kind of a grand generalization of Bang’s theorem, with effective bounds on the exceptional cases.) These results should give an effective version of Zsigmondy’s theorem for $\mathbb{Q}[i]$, which would provide an exclusion criterion for Machin-type BBP arctangent formulae that would be analogous to Theorem 6.
- (9) For the binary case, can we find exclusion criteria that deal with Aurifeuillian generators in logarithm formulae?
- (10) We could generalize the definition of a BBP-formula to allow sums of the form $\sum_{k \geq 0} b^{-k} p(k)/q(k)$, $b \in \mathbb{Z}[i]$, $p, q \in \mathbb{Z}[i, k]$. Doing so should avoid the need to treat arctangents and logarithms as separate cases. Could we get cleaner or more general results this way?
- (11) Let ζ_n denote a primitive n th root of unity, and recall that $L(s, b, n, A)$ is defined by Equation (3). It’s a simple exercise to show that for $1 \leq j \leq n$ we have

$$(63) \quad L(1, b, n, j) = -\frac{1}{n} b^{j/n} \sum_{r=0}^{n-1} \zeta_n^{-rj} \ln(1 - \zeta_n^r b^{-1/n}).$$

(In his answer to [Knu98, Exercise 4.3.1.39], Knuth gives a different version of an explicit formula for $L(1, b, n, j)$.) Can our techniques be applied to determine whether or not a constant κ may be written as a linear combination of $L(1, b^m, n, j)$, with b , and perhaps n , fixed? This would probably require a good understanding of the algebraic number field $\mathbb{Q}[\zeta_n, b^{1/n}]$, among other things.

- (12) To what extent can we justify the idea that our limited set of “Machin-type” BBP generators gives all (or most) “interesting” arctangents and logarithms?

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