A Class of Conjectured Series Representations for $1/\pi$

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CONTENTS

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Using the second conjecture in the paper [Guillera 06b] and inspired by the theory of modular functions, we find a method that allows us to obtain explicit formulas, involving eta or theta functions, for the parameters of a class of series for $1/\pi$. As in [Guillera 06b], the series considered in this paper include Ramanujan's series as well as those associated with the Domb numbers and Apéry numbers.

1. A SPECIAL TYPE OF RECURRENCE

The sequence of integers

$$B_n = \frac{(2n)!^3}{n!^6} \tag{1–1}$$

satisfies the following recurrence:

$$n^3 B_n - 8(2n-1)^3 B_{n-1} = 0.$$

Other sequences of integers satisfying a first-order recurrence whose coefficients are third degree-polynomials,

$$B_n = \frac{(4n)!}{n!^4}, \tag{1–2}$$

$$B_n = \frac{(2n)!(3n)!}{n!^5}, \tag{1–3}$$

and

$$B_n = \frac{(6n)!}{(3n)!n!^3}, \tag{1–4}$$

satisfy the recurrences

$$n^3 B_n - 8(2n-1)(4n-3)(4n-1)B_{n-1} = 0,$$
$$n^3 B_n - 6(2n-1)(3n-2)(3n-1)B_{n-1} = 0,$$

and

$$n^3 B_n - 24(2n-1)(6n-5)(6n-1)B_{n-1} = 0,$$

respectively. Examples of sequences of integers that satisfy a second-order recurrence with third-degree polynomials as coefficients are [Almkvist and Zudilin 03] the sequence of Domb numbers [Chan et al. 04]

$$B_n = \sum_{j=0}^{n} \binom{n}{j}^2 \binom{2j}{j} \binom{2n-2j}{n-j}, \tag{1–5}$$

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which satisfy

$$n^3B_n-2(2n-1)(5n^2-5n+2)B_{n-1}+64(n-1)^3B_{n-2}=0; \tag{1–6}$$

the sequence of Apéry numbers

$$B_n=\sum_{j=0}^{n}\binom{n}{j}^2\binom{n+j}{j}^2, \tag{1–7}$$

which satisfy

$$n^3B_n-(2n-3)(17n^2-17n+5)B_{n-1}+(n-1)^3B_{n-2}=0;$$

and the sequences

$$B_n=\sum_{j=0}^{n}\binom{n}{j}^4 \tag{1–8}$$

and

$$B_n=\sum_{j=0}^{\lfloor n/3\rfloor}3^{n-3j}\binom{n}{3j}\binom{n+j}{j}\frac{(3j)!}{j!^3}, \tag{1–9}$$

which satisfy similar recurrences. Our interest in sequences of integers B_n satisfying a recurrence with third-degree polynomials as coefficients comes from the fact that for certain of them [Almkvist and Zudilin 03] there exist algebraic numbers z, a, and b such that

$$\sum_{n=0}^{\infty}B_nz^n(a+bn)=\frac{1}{\pi}. \tag{1–10}$$

Series for $1/\pi$ associated with the sequences in (1–1), (1–2), (1–3), and (1–4) were first discovered by Ramanujan and were extensively studied later. Proofs can be found in [Berndt and Chan 01, Borwein and Borwein 87, Chan et al. 01, Chudnovsky and Chudnovsky 87, Ramanujan 14]. In [Guillera 06a] the author gave simpler proofs of some identities of the form (1–10) using the WZ method. Series for $1/\pi$ using the Apéry numbers (1–7) were presented in a talk of T. Sato [Sato 02]. Motivated by them, similar series for $1/\pi$ associated with the Domb numbers (1–5) have been studied and proved in [Chan et al. 04]. H. H. Chan [Chan 05], also gives some examples of series for $1/\pi$ associated with several sequences, one of them with the numbers (1–9). Y. Yang has proved similar evaluations [Yang 05] using the numbers (1–8) and following a technique explained in [Yang 04]. Other sequences satisfying recurrences with third-degree polynomials as coefficients [Almkvist and Zudilin 03] will be used in the examples of Section 4.

2. A COMPANION SEQUENCE

To each B_n, we associate a companion D_n defined by

$$D_n=\frac{dB_n}{dn},$$

where d/dn means that we differentiate as if n were a continuous variable. From the recurrence of B_n we can obtain a recurrence for D_n. For example, the recurrence (1–6) for the Domb numbers (1–5) can be written in the form

$$B_n=2\frac{(2n-1)(5n^2-5n+2)}{n^3}B_{n-1}-64\frac{(n-1)^3}{n^3}B_{n-2},$$

and differentiating with respect to n as if n were a continuous variable, we obtain

$$\begin{aligned}D_n&=2\frac{(2n-1)(5n^2-5n+2)}{n^3}D_{n-1}-64\frac{(n-1)^3}{n^3}D_{n-2}\\&\quad+6\frac{5n^2-6n+2}{n^4}B_{n-1}-192\frac{(n-1)^2}{n^4}B_{n-2}.\end{aligned}$$

From the initial conditions $B_0=1$ and $D_0=0$, we get

$$B_1=4B_0+0B_{-1}=4, \tag{2–1}$$

$$D_1=4D_0+0D_{-1}+6B_0+0B_{-1}=6, \tag{2–2}$$

and with those values and using the recurrences, we can determine $B_2, B_3, \dots$ and $D_2, D_3, \dots$.

3. TWO CONJECTURES

In this section we give a method and two conjectures that will allow us to obtain explicit formulas involving eta or theta functions for the parameters of a class of series for $1/\pi$.

Motivated by the theory of modular functions we begin by introducing the variable

$$q=e^{-\pi\sqrt{N}}. \tag{3–1}$$

Now, inspired by the paper [Guillera 06b], we define the functions

$$S(z)=\sum_{n=0}^{\infty}B_nz^n \tag{3–2}$$

and

$$W(z)=\sum_{n=0}^{\infty}\frac{dB_n}{dn}z^n=\sum_{n=0}^{\infty}D_nz^n$$

and consider the following equation relating z and q:

$$q=z\exp\frac{W(z)}{S(z)}. \tag{3–3}$$

If we write z as a series of powers of q,

$$z = \alpha_1 q + \alpha_2 q^2 + \alpha_3 q^3 + \alpha_4 q^4 + \cdots, \qquad (3\text{–}4)$$

then the coefficients are given by

$$\begin{aligned} \alpha_1 &= \lim_{z\to 0} \frac{z}{q}, \\ \alpha_2 &= \lim_{z\to 0} \frac{z-\alpha_1 q}{q^2}, \\ \alpha_3 &= \lim_{z\to 0} \frac{z-\alpha_1 q - \alpha_2 q^2}{q^3} \\ &\vdots \end{aligned} \qquad (3\text{–}5)$$

In the same way, if we write S as a series of powers of q,

$$S = 1 + \beta_1 q + \beta_2 q^2 + \beta_3 q^3 + \beta_4 q^4 + \cdots, \qquad (3\text{–}6)$$

the coefficients are given by

$$\begin{aligned} \beta_1 &= \lim_{z\to 0} \frac{S-1}{q}, \\ \beta_2 &= \lim_{z\to 0} \frac{S-1-\beta_1 q}{q^2}, \\ \beta_3 &= \lim_{z\to 0} \frac{S-1-\beta_1 q - \beta_2 q^2}{q^3} \\ &\vdots \end{aligned} \qquad (3\text{–}7)$$

Conjecture 3.1. *The coefficients of (3–4) and (3–6), given by (3–5) and (3–7), are all integers, and z and S are the products of a finite number of Dedekind η functions:*

$$\eta(q) = q^{1/24} \prod_{n=0}^{\infty} (1-q^{n+1}).$$

Furthermore, for some rational values of N, z is an algebraic number.

We define the function

$$V(z) = \sum_{n=0}^{\infty} \frac{d}{dn}(B_n z^n) = W(z) + \ln(z) S(z).$$

From (3–1) and (3–3), we get the equation

$$\frac{V(z)}{S(z)} = -\pi\sqrt{N}. \qquad (3\text{–}8)$$

Inspired by the paper [Guillera 06b], we consider the equations

$$aS + bz\frac{dS}{dz} = \frac{1}{\pi}, \qquad (3\text{–}9)$$

$$aV + bz\frac{dV}{dz} = 0. \qquad (3\text{–}10)$$

From (3–8) and (3–10) we get

$$a(\ln q)S + bz\frac{d}{dz}\left[(\ln q)S\right] = 0, \qquad (3\text{–}11)$$

and using (3–11) we obtain

$$a(\ln q)S + bz\left[\frac{1}{q}\left(\frac{dz}{dq}\right)^{-1} S + (\ln q)\frac{dS}{dz}\right] = 0. \qquad (3\text{–}12)$$

From (3–12) and (3–9) we obtain the following formula, which allows us to determine the parameter b:

$$\frac{b}{\sqrt{N}} = \frac{q}{zS}\frac{dz}{dq}. \qquad (3\text{–}13)$$

Using (3–9), we get the following formula for the parameter a:

$$a = \frac{1}{S}\left(\frac{1}{\pi} - bz\frac{dS}{dz}\right) = \frac{1}{S}\left[\frac{1}{\pi} - bz\frac{dS}{dq}\left(\frac{dz}{dq}\right)^{-1}\right],$$

which, with the use of (3–13), gives

$$a = \frac{1}{S}\left[\frac{1}{\pi} - \frac{q\sqrt{N}}{S}\frac{dS}{dq}\right], \qquad (3\text{–}14)$$

which allows us to determine the parameter a.

Conjecture 3.2. *Substituting the values of z and S in (3–13) and (3–14) we obtain values for a and b such that the following identity holds:*

$$\sum_{n=0}^{\infty} B_n z^n (a+bn) = \frac{1}{\pi}. \qquad (3\text{–}15)$$

Moreover, for the rational values of N for which z is an algebraic number (see Conjecture 3.1), the parameters a and b are also algebraic numbers.

4. EXAMPLES

Example 4.1. We take the sequence of numbers

$$B_n = \sum_{j=0}^{n} \binom{2j}{j}^2 \binom{2n-2j}{n-j}^2.$$

The numbers B_n are obtained recursively by setting $B_0 = 1$ and

$$B_n = 8\frac{(2n-1)(2n^2-2n+1)}{n^3}B_{n-1} - 256\frac{(n-1)^3}{n^3}B_{n-2}.$$

Although this is a second-order recurrence, we can obtain B_1 as in (2–1). The companions D_n satisfy the recurrence $D_0 = 0$ and

$$D_n = 8\frac{(2n-1)(2n^2-2n+1)}{n^3}D_{n-1} - 256\frac{(n-1)^3}{n^3}D_{n-2} + 8\frac{6n^2-8n+3}{n^4}B_{n-1} - 768\frac{(n-1)^2}{n^4}B_{n-2},$$

and again, we obtain D_1 as in (2–2). Following the method described in Section 3, we get

$$z = q - 8q^2 + 44q^3 - 192q^4 + 718q^5 - 2400q^6 + 7352q^7 - 20992q^8 + \cdots,$$
$$S = 1 + 8q + 24q^2 + 32q^3 + 24q^4 + 48q^5 + 96q^6 + 64q^7 + 28q^8 + \cdots.$$

Searching the sequences of the coefficients of these series in the *On-Line Encyclopedia of Integer Sequences* [Sloane 06], we find that

$$z = \frac{\theta_2^4(q)}{16\theta_3^4(q)} = \frac{\lambda^*(q)^2}{16} \qquad (4\text{–}1)$$

and

$$S = \theta_3^4(q), \qquad (4\text{–}2)$$

where $\theta_2(q)$ and $\theta_3(q)$ are Jacobi theta functions and $\lambda^*(q)$ is the elliptic lambda modulus function, defined by

$$\lambda^*(q) = \frac{\theta_2^2(q)}{\theta_3^2(q)}.$$

Substituting in (3–2) the values given in (4–1) and (4–2), we obtain the formula

$$\theta_3^4(q) = \sum_{n=0}^{\infty} B_n \left(\frac{\theta_2^4(q)}{16\theta_3^4(q)}\right)^n.$$

Substituting (4–1) and (4–2) in (3–13) and expanding in a power series of q, we get

$$\frac{b}{\sqrt{N}} = 1 - 16q + 128q^2 - 704q^3 + 3072q^4 - 11488q^5 + 38400q^6 - \cdots.$$

Again using the *On-Line Encyclopedia of Integer Sequences* [Sloane 06], we are lucky and find that

$$\frac{b}{\sqrt{N}} = 1 - \frac{\theta_2^4(q)}{\theta_3^4(q)} = 1 - \lambda^*(q)^2 = \frac{\theta_4^4(q)}{\theta_3^4(q)}. \qquad (4\text{–}3)$$

Substituting (4–2) in (3–14), we obtain

$$a = \frac{\frac{1}{\pi} - 4\sqrt{N}q\frac{1}{\theta_3(q)}\frac{d\theta_3(q)}{dq}}{\theta_3^4(q)} = \alpha(-q)[1-\lambda^*(q)^2], \qquad (4\text{–}4)$$

where $\alpha(q)$ is the elliptic alpha function, defined by

$$\alpha(q) = \frac{\frac{1}{\pi} - 4\sqrt{N}q\frac{1}{\theta_4(q)}\frac{d\theta_4(q)}{dq}}{\theta_3^4(q)}.$$

Substituting in (3–15) the values of the parameters given in (4–1), (4–3), and (4–4), we obtain the following formula:

$$\frac{1}{\pi} = [1-\lambda^*(q)^2]\sum_{n=0}^{\infty} B_n \left(\frac{\lambda^*(q)^2}{16}\right)^n \left[\alpha(-q) + \sqrt{N}n\right],$$

where $q = e^{-\pi\sqrt{N}}$ or $q = -e^{-\pi\sqrt{N}}$.

Example 4.2. We take the numbers defined recursively by $B_0 = 1$ and

$$B_n = 4\frac{(2n-1)(3n^2-3n+1)}{n^3}B_{n-1} - 16\frac{(n-1)^3}{n^3}B_{n-2}.$$

The companions D_n satisfy the recurrence $D_0 = 0$ and

$$D_n = 4\frac{(2n-1)(3n^2-3n+1)}{n^3}D_{n-1} - 16\frac{(n-1)^3}{n^3}D_{n-2} + 4\frac{9n^2-10n+3}{n^4}B_{n-1} - 48\frac{(n-1)^2}{n^4}B_{n-2}.$$

Following the method described in Section 3, we get

$$z = q - 8q^2 + 28q^3 - 64q^4 + 142q^5 - 352q^6 + 792q^7 - 1536q^8 + 2917q^9 - 5744q^{10} + \cdots$$

and

$$S = 1 + 4q + 8q^2 + 16q^3 + 24q^4 + 24q^5 + 32q^6 + 32q^7 + 24q^8 + 52q^9 + 48q^{10} \cdots.$$

With the *On-Line Encyclopedia of Integer Sequences*, we find that

$$S = \theta_3^2(q)\theta_3^2(q^2). \qquad (4\text{–}5)$$

Using the Maple package *q-series* [Garvan 05], more specifically the functions *prodmake* and *etamake*, we find that

$$z = q\prod_{n=0}^{\infty}\left(\frac{1-q^{2n+1}}{1-q^{8n+4}}\right)^8 = \left[\frac{\eta(q^8)}{\eta(q^2)}\frac{\eta(q)}{\eta(q^4)}\right]^8. \qquad (4\text{–}6)$$

From the identities [Garvan 05]

$$\theta_2(q) = 2\frac{\eta^2(q^4)}{\eta(q^2)},$$
$$\theta_3(q) = \frac{\eta^5(q^2)}{\eta^2(q^4)\,\eta^2(q)}, \qquad (4\text{–}7)$$
$$\theta_4(q) = \frac{\eta^2(q)}{\eta(q^2)},$$

we can get

$$\eta(q) = \left[\frac{1}{2}\theta_2(q)\theta_3(q)\theta_4^4(q)\right]^{1/6}, \qquad (4–8)$$

which allows us to convert formulas using the Dedekind eta function into formulas using the Jacobi theta functions θ_2, θ_3, and θ_4. From (4–6) and using (4–8), we can express z with θ functions. A more simplified formula is

$$z = \left[\frac{\theta_2(q^2)}{\theta_2(q)}\frac{\theta_4(q)}{\theta_4(q^2)}\right]^4, \qquad (4–9)$$

which can be obtained using the first and third identities of (4–7). Substituting (4–5) and (4–9) in (3–2), we obtain the formula

$$\sum_{n=0}^{\infty} B_n \left[\frac{\theta_2(q^2)}{\theta_2(q)}\frac{\theta_4(q)}{\theta_4(q^2)}\right]^{4n} = \theta_3^2(q)\theta_3^2(q^2).$$

Taking the logarithm of (4–6) and differentiating with respect to q, we get

$$\frac{q}{z}\frac{dz}{dq} = 1 + 8\sum_{n=0}^{\infty}\frac{(2n+1)q^{2n+1}}{1-q^{2n+1}} - 8\sum_{n=0}^{\infty}\frac{(8n+4)q^{8n+4}}{1-q^{8n+4}}. \qquad (4–10)$$

From the formula (3.2.24) of [Borwein and Borwein 87] and the identities $\theta_4(-q) = \theta_3(q)$ and $\theta_2^4(-q) = -\theta_2^4(q)$, we get

$$\theta_2^4(q) + \theta_3^4(q) = 1 + 24\sum_{n=0}^{\infty}\frac{(2n+1)q^{2n+1}}{1-q^{2n+1}},$$

which allows us to write (4–10) using θ functions:

$$\frac{q}{z}\frac{dz}{dq} = \frac{4\theta_2^4(q^4) + 4\theta_3^4(q^4) - \theta_2^4(q) - \theta_3^4(q)}{3}. \qquad (4–11)$$

Substituting (4–5) and (4–11) in (3–13), we obtain

$$\frac{b}{\sqrt{N}} = \frac{4\theta_2^4(q^4) + 4\theta_3^4(q^4) - \theta_2^4(q) - \theta_3^4(q)}{3\theta_3^2(q)\theta_3^2(q^2)}. \qquad (4–12)$$

Substituting (4–5) in (3–14), we obtain

$$a = \frac{\frac{1}{\pi} - 2\sqrt{N}q\left(\frac{1}{\theta_3(q)}\frac{d\theta_3(q)}{dq} + \frac{1}{\theta_3(q^2)}\frac{d\theta_3(q^2)}{dq}\right)}{\theta_3^2(q)\theta_3^2(q^2)}. \qquad (4–13)$$

Substituting in (3–15) the values of the parameters z, b, and a given by (4–9), (4–12), and (4–13), we obtain a family of series for $1/\pi$.

Example 4.3. We take the numbers defined recursively by $B_0 = 1$ and

$$B_n = 3\frac{(2n-1)(3n^2-3n+1)}{n^3}B_{n-1} + 27\frac{(n-1)^3}{n^3}B_{n-2}.$$

The companions D_n satisfy the recurrence $D_0 = 0$ and

$$D_n = 3\frac{(2n-1)(3n^2-3n+1)}{n^3}D_{n-1} + 27\frac{(n-1)^3}{n^3}D_{n-2} + 3\frac{9n^2-10n+3}{n^4}B_{n-1} + 81\frac{(n-1)^2}{n^4}B_{n-2}.$$

Following the method in Section 3, we get

$$z = q - 6q^2 + 9q^3 + 22q^4 - 102q^5 + 108q^6 + 221q^7 + 7802q^{13} - 858q^8 + 810q^9 + 1476q^{10} - 5262q^{11} + 4572q^{12} - 26112q^{14} + 21519q^{15} + \cdots$$

and

$$S = 1 + 3q + 9q^2 + 12q^3 + 21q^4 + 18q^5 + 36q^6 + 24q^7 + 45q^8 + 12q^9 + \cdots.$$

Using the Maple package *q-series* [Garvan 05], more specifically the functions *prodmake* and *etamake*, we find that

$$z = q\prod_{n=0}^{\infty}\frac{(1-q^{n+1})^6(1-q^{9n+9})^6}{(1-q^{3n+3})^{12}} = \left[\frac{\eta(q)\,\eta(q^9)}{\eta^2(q^3)}\right]^6 \qquad (4–14)$$

and

$$S = \prod_{n=0}^{\infty}\frac{(1-q^{3n+3})^{10}}{(1-q^{n+1})^3(1-q^{9n+9})^3} = \frac{\eta^{10}(q^3)}{\eta^3(q)\,\eta^3(q^9)}. \qquad (4–15)$$

The expressions of z and S allow us to write the formula

$$\sum_{n=0}^{\infty} B_n\left[\frac{\eta(q)\,\eta(q^9)}{\eta^2(q^3)}\right]^{6n} = \frac{\eta^{10}(q^3)}{\eta^3(q)\,\eta^3(q^9)}.$$

And substituting in

$$\sum_{n=0}^{\infty} B_n z^n\left[\frac{1}{S}\left(\frac{1}{\pi} - \frac{q\sqrt{N}}{S}\frac{dS}{dq}\right) + \frac{q\sqrt{N}}{zS}\frac{dz}{dq}n\right] = \frac{1}{\pi}$$

the values of z and S given in (4–14) and (4–15), we obtain another family of series for $1/\pi$.

Example 4.4. It seems that Conjecture 3.1 (but not Conjecture 3.2) remains true when we consider certain sequences of integers satisfying recurrences whose coefficients are second-degree polynomials [Almkvist and Zudilin 03]. As an example we take the sequence of integers [Almkvist and Zudilin 03]

$$B_n = \sum_{k=0}^{n}\binom{n}{k}\binom{2k}{k}\binom{2n-2k}{n-k}.$$

This sequence satisfies the recurrence $B_0 = 1$ and

$$B_n = \frac{4(3n^2 - 3n + 1)}{n^2} B_{n-1} - \frac{32(n-1)^2}{n^2} B_{n-2}.$$

The companion numbers D_n satisfy the recurrence $D_0 = 0$ and

$$D_n = \frac{4(3n-2)}{n^3} B_{n-1} - \frac{64(n-1)}{n^3} B_{n-2} + \frac{4(3n^2 - 3n + 1)}{n^2} D_{n-1} - \frac{32(n-1)^2}{n^2} D_{n-2}.$$

Following the procedure in Section 3, we get

$$z = q - 4q^2 + 12q^3 - 32q^4 + 78q^5 - 176q^6 + 376q^7 - 768q^8 + 1509q^9 - 2872q^{10} + \cdots$$

and

$$S = 1 + 4q + 4q^2 + 4q^4 + 8q^5 + 4q^8 + 4q^9 + 8q^{10} + \cdots .$$

Searching the sequences of the coefficients of these series in the *On-Line Encyclopedia of Integer Sequences* [Sloane 06], we are lucky and find that

$$z = \left[\frac{\eta^2(q^8)}{\eta(q^4)} \right]^2 \left[-\frac{\eta(q^2)}{\eta^2(-q)} \right]^{-2} = \frac{\theta_2^2(q^2)}{4\theta_3^2(q)}$$

and

$$S = \theta_3^2(q),$$

which allows us to write the formula

$$\sum_{n=0}^{\infty} B_n \left[\frac{\theta_2^2(q^2)}{4\theta_3^2(q)} \right]^n = \theta_3^2(q).$$

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