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Series and iterations for $1/\pi$

by

SHAUN COOPER (Auckland)

1. Introduction. H. H. Chan and K. P. Loo [14] used properties of Ramanujan's cubic continued fraction to establish the following series for $1/\pi$:

$$\frac{\sqrt{6}}{2\pi} = (1+w_3)(1-8w_3)\sum_{k=0}^{\infty} C_3(k)\left(k+\frac{w_3}{1+w_3}\right)w_3^k \tag{1.1}$$

where

$$C_3(k) = \sum_{j=0}^{k} c_3(j)c_3(k-j), \qquad c_3(k) = \sum_{j=0}^{k}\binom{k}{j}^3, \qquad w_3 = \frac{3\sqrt{2}}{4}-1.$$

In this work, we shall establish the series:

$$\frac{\sqrt{6}}{2\pi} = (1-w_2)(1-9w_2)\sum_{k=0}^{\infty} C_2(k)\left(k-\frac{w_2}{1-w_2}\right)w_2^k, \tag{1.2}$$

$$\frac{\sqrt{4}}{2\pi} = (1-16w_4)^2\sum_{k=0}^{\infty} C_4(k)\left(k-\frac{16w_4}{1-16w_4}\right)w_4^k \tag{1.3}$$

and

$$\frac{\sqrt{5}}{2\pi} = (1-11w_5-w_5^2)\sum_{k=0}^{\infty} C_5(k)\left(k+\frac{\gamma^5 w_5}{1+\gamma^5 w_5}\right)w_5^k \tag{1.4}$$

where

$$C_n(k) = \sum_{j=0}^{k} c_n(j)c_n(k-j) \qquad \text{for } n = 2, 4 \text{ or } 5,$$

$$c_2(k) = \sum_{j=0}^{k}\binom{k}{j}^2\binom{2j}{j}, \qquad w_2 = 1-\frac{\sqrt{8}}{3},$$

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$$c_4(k)=\sum_{j=0}^{k}\binom{2j}{j}^2\binom{2k-2j}{k-j}2^{2k-2j},\qquad w_4=\frac{1}{32},$$

$$c_5(k)=\sum_{j=0}^{k}\binom{k}{j}^2\binom{k+j}{j},\qquad w_5=\frac{1}{\gamma^5}(\sqrt{1+\gamma^{10}}-1),\qquad \gamma=\frac{\sqrt{5}-1}{2}.$$

It will be shown that each of the series (1.1)–(1.4) yields approximately one binary digit per term, i.e., about 0.3 decimal places per term. Although we have given explicit formulas for the coefficients $C_n(k)$ as multiple sums of binomial coefficients, the coefficients $C_2(k)$, $C_3(k)$, $C_4(k)$ and $C_5(k)$ all satisfy third order linear recurrence relations, which are more suitable for computation.

We shall also establish five iterations for $1/\pi$, two of which are new.

Behind these series and iterations for $1/\pi$ are modular forms for the spaces $\Gamma_0(4)$, $\Gamma_0(5)$, $\Gamma_0(6)$ and $\Gamma_0(8)$ (see, e.g., [19]). Our development relies heavily on properties of the Ramanujan–Selberg, Rogers–Ramanujan, cubic Ramanujan and Ramanujan–Göllnitz–Gordon continued fractions. We develop the theory of these functions from scratch, as much as possible, using properties of theta functions and the modular transformation for Dedekind's eta function.

This work is motivated by the paper [14] and the author is indebted to Prof. H. H. Chan for introducing him to this topic in a series of lectures given at Massey University in 2005.

2. Notation and basic lemmas. Let τ be a complex number with positive imaginary part and put $q=\exp(2\pi i\tau)$, so that $|q|<1$. When τ is purely imaginary, write $\tau=it$, where t is a positive real number, so that $q=\exp(-2\pi t)$.

Dedekind's eta function is defined by

$$\eta(\tau)=q^{1/24}\prod_{j=1}^{\infty}(1-q^j).$$

It satisfies the transformation formula [2, pp. 43–44], [19, (7.1)]

$$\eta(\tau)=\sqrt{\frac{i}{\tau}}\,\eta\left(-\frac{1}{\tau}\right)\tag{2.1}$$

and has the Fourier expansion [4, p. 12]

$$\eta(\tau)=q^{1/24}\sum_{j=-\infty}^{\infty}(-1)^j q^{j(3j-1)/2}=\sum_{j=-\infty}^{\infty}(-1)^j q^{(6j-1)^2/24}.\tag{2.2}$$

Ramanujan's theta functions are defined by

$$\varphi(q) = \sum_{j=-\infty}^{\infty} q^{j^2} \quad \text{and} \quad \psi(q) = \sum_{j=0}^{\infty} q^{j(j+1)/2}.$$

They have the infinite product representations [4, p. 11]

$$\varphi(q) = \frac{\eta^5(2\tau)}{\eta^2(\tau)\eta^2(4\tau)}, \qquad \varphi(-q) = \frac{\eta^2(\tau)}{\eta(2\tau)}, \qquad q^{1/8}\psi(q) = \frac{\eta^2(2\tau)}{\eta(\tau)}, \tag{2.3}$$

and satisfy the well-known properties [2, p. 40], [4, pp. 71–72]

$$\varphi(q^4) = \varphi(-q) + 2q\psi(q^8), \tag{2.4}$$

$$2\varphi^2(q^2) = \varphi^2(q) + \varphi^2(-q), \tag{2.5}$$

$$8q\psi^2(q^4) = \varphi^2(q) - \varphi^2(-q), \tag{2.6}$$

$$16q\psi^4(q^2) = \varphi^4(q) - \varphi^4(-q). \tag{2.7}$$

We shall also use the lesser-known properties

$$q^{1/2}\psi^2(q^2) + q^{3/2}\psi^2(q^6) = \frac{\eta^3(3\tau)\eta(4\tau)\eta(12\tau)}{\eta(\tau)\eta^2(6\tau)}, \tag{2.8}$$

$$q^{1/2}\psi^2(q^2) - 3q^{3/2}\psi^2(q^6) = \frac{\eta^3(\tau)\eta(4\tau)\eta(12\tau)}{\eta^2(2\tau)\eta(3\tau)}. \tag{2.9}$$

The first of these is equivalent to [3, p. 110, Lemma 5.3] and the second may easily be proved by the same methods as in [3, p. 110].

The Borweins' cubic theta functions a, b and c are defined by

$$\begin{aligned} a(q) &= \sum_j \sum_k q^{j^2+jk+k^2}, \\ b(q) &= \sum_j \sum_k w^{j-k} q^{j^2+jk+k^2}, \qquad \text{where } w = \exp(2\pi i/3), \\ c(q) &= \sum_j \sum_k q^{(j+\frac{1}{3})^2+(j+\frac{1}{3})(k+\frac{1}{3})+(k+\frac{1}{3})^2}, \end{aligned}$$

where the sums range over all integer values of j and k. The functions b and c have the infinite product expansions [3, p. 109], [21], [22]

$$b(q) = \frac{\eta^3(\tau)}{\eta(3\tau)} \quad \text{and} \quad c(q) = 3\,\frac{\eta^3(3\tau)}{\eta(\tau)} \tag{2.10}$$

and the function a has a Lambert series expansion [3, p. 93], [8], [22]

$$a(q) = 1 + 6\sum_{j=1}^{\infty}\left(\frac{q^{3j-2}}{1-q^{3j-2}} - \frac{q^{3j-1}}{1-q^{3j-1}}\right). \tag{2.11}$$

3. The functions u_n, v_n, w_n and x_n. Let

$$u_2 = u_2(q) = q^{1/2}\prod_{j=1}^{\infty}\frac{(1-q^{6j-5})^2(1-q^{6j-1})^2}{(1-q^{6j-4})^2(1-q^{6j-2})^2} = \frac{\eta^2(\tau)\eta^4(6\tau)}{\eta^4(2\tau)\eta^2(3\tau)},$$

$$u_3 = u_3(q) = q^{1/3}\prod_{j=1}^{\infty}\frac{(1-q^{6j-5})(1-q^{6j-1})}{(1-q^{6j-3})^2} = \frac{\eta(\tau)\eta^3(6\tau)}{\eta(2\tau)\eta^3(3\tau)},$$

$$u_4 = u_4(q) = q^{1/4}\prod_{j=1}^{\infty}\frac{(1-q^{4j-3})^2(1-q^{4j-1})^2}{(1-q^{4j-2})^4} = \frac{\eta^2(\tau)\eta^4(4\tau)}{\eta^6(2\tau)},$$

$$u_5 = u_5(q) = q^{1/5}\prod_{j=1}^{\infty}\frac{(1-q^{5j-4})(1-q^{5j-1})}{(1-q^{5j-3})(1-q^{5j-2})}.$$

The functions u_3, $u_4^{1/2}$ and u_5 have expansions as continued fractions. These are usually referred to as Ramanujan's cubic continued fraction, the Ramanujan–Selberg continued fraction and the Rogers–Ramanujan continued fraction, respectively. I do not know of a continued fraction for u_2 (or for $u_2^{1/2}$), but it is related to Ramanujan's cubic continued fraction by ([1])

$$\frac{1}{u_2^2} - \frac{1}{u_3^3} = 1. \tag{3.1}$$

Another continued fraction—the Ramanujan–Göllnitz–Gordon continued fraction—will be encountered in Section 8. For more information about these continued fractions and references to other sources, see [1] and [19].

For $n = 2, 3, 4$ or 5, let

$$v_n = v_n(q) = u_n(q^n) \quad\text{and}\quad w_n = w_n(q) = u_n^n(q).$$

Let

$$x_2 = x_2(q) = \frac{\eta^6(2\tau)\eta^6(6\tau)}{\eta^6(\tau)\eta^6(3\tau)}, \qquad x_3 = x_3(q) = \frac{\eta^4(3\tau)\eta^4(6\tau)}{\eta^4(\tau)\eta^4(2\tau)},$$

$$x_4 = x_4(q) = \frac{\eta^{24}(2\tau)}{\eta^{24}(\tau)}, \qquad x_5 = x_5(q) = \frac{\eta^6(5\tau)}{\eta^6(\tau)}.$$

Let $\gamma = (\sqrt{5}-1)/2$.

([1]) The identity (3.1) is equivalent to

$$\frac{\psi^3(q)}{\psi(q^3)} - \frac{\varphi^3(-q^3)}{\varphi(-q)} = q\,\frac{\psi^3(q^3)}{\psi(q)}$$

and this can be proved by expanding each side as Lambert series by the techniques in [4, Theorem 6.3.3]. Alternatively, the identity (3.1) can be proved using properties of Hauptmoduls.

The starting point of the theory is

THEOREM 3.1. *For $n = 2, 3, 4$ or 5, and with u_n, w_n and x_n as defined above,*

$$\begin{aligned} \frac{1}{u_2} - 2 - 3u_2 &= \frac{\eta^2(\tau/2)\eta^2(3\tau/2)}{\eta^2(2\tau)\eta^2(6\tau)}, & \frac{1}{w_2} - 10 + 9w_2 &= \frac{1}{x_2}, \\ \frac{1}{u_3} - 1 - 2u_3 &= \frac{\eta(\tau/3)\eta(2\tau/3)}{\eta(3\tau)\eta(6\tau)}, & \frac{1}{w_3} - 7 - 8w_3 &= \frac{1}{x_3}, \\ \frac{1}{u_4} - 4u_4 &= \frac{\eta^4(\tau/2)}{\eta^4(2\tau)}, & \frac{1}{w_4} - 32 + 256w_4 &= \frac{1}{x_4}, \\ \frac{1}{u_5} - 1 - u_5 &= \frac{\eta(\tau/5)}{\eta(5\tau)}, & \frac{1}{w_5} - 11 - w_5 &= \frac{1}{x_5}. \end{aligned}$$

Proof. Let us prove the results that involve u_n first.

By (2.8) and (2.9), we have

$$\begin{aligned} \frac{1}{u_2} - 2 - 3u_2 &= \frac{1}{u_2}(1+u_2)(1-3u_2) \\ &= \frac{\eta^2(\tau)\eta^2(3\tau)}{\eta^4(2\tau)\eta^4(6\tau)}(q^{1/4}\psi^2(q) + q^{3/4}\psi^2(q^3))(q^{1/4}\psi^2(q) - 3q^{3/4}\psi^2(q^3)) \\ &= \frac{\eta^2(\tau)\eta^2(3\tau)}{\eta^4(2\tau)\eta^4(6\tau)} \cdot \frac{\eta^3(3\tau/2)\eta(2\tau)\eta(6\tau)}{\eta(\tau/2)\eta^2(3\tau)} \cdot \frac{\eta^3(\tau/2)\eta(2\tau)\eta(6\tau)}{\eta^2(\tau)\eta(3\tau/2)} \\ &= \frac{\eta^2(\tau/2)\eta^2(3\tau/2)}{\eta^2(2\tau)\eta^2(6\tau)}, \end{aligned}$$

and this proves the result for u_2.

To prove the result for u_3, we expand $\prod_{j=1}^{\infty}(1-q^j)(1-q^{2j})$ as a double series using (2.2), and trisect using the series rearrangement

$$\sum_{m,n} c_{m,n} = \sum_{j,k} c_{j+2k,j-k} + \sum_{j,k} c_{j+2k+1,j-k} + \sum_{j,k} c_{j+2k,j-k+1}.$$

We find that

$$\begin{aligned} \prod_{j=1}^{\infty}(1-q^j)(1-q^{2j}) &= \sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}(-1)^{m+n}q^{m(3m-1)/2+n(3n-1)} \\ &= \sum_{j=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}(-1)^k q^{9k^2+3j(3j-1)/2} \\ &\quad - q\sum_{j=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}(-1)^k q^{9k^2+6k+3j(3j+1)/2} \\ &\quad - q^2\sum_{j=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}(-1)^k q^{9k^2-6k+9j(j+1)/2}. \end{aligned}$$

Now apply the Jacobi triple product identity [4, p. 10] to each sum, and simplify the resulting infinite products, to get

$$\prod_{j=1}^{\infty}(1-q^j)(1-q^{2j}) = \prod_{j=1}^{\infty}\frac{(1-q^{6j})(1-q^{9j})^4}{(1-q^{3j})(1-q^{18j})^2} - q\prod_{j=1}^{\infty}(1-q^{9j})(1-q^{18j}) - 2q^2\prod_{j=1}^{\infty}\frac{(1-q^{3j})(1-q^{18j})^4}{(1-q^{6j})(1-q^{9j})^2}.$$

Divide both sides by $\prod_{j=1}^{\infty}(1-q^{9j})(1-q^{18j})$ and replace q^3 with q to obtain the result for u_3.

To prove the result for u_4, note that from (2.5) and (2.6) we have

$$\varphi^2(-q^{1/2}) = \varphi^2(q) - 4q^{1/2}\psi^2(q^2).$$

Therefore, on using (2.3) we get

$$\begin{aligned}\frac{1}{u_4} - 4u_4 &= \frac{\eta^2(\tau)}{\eta^4(2\tau)}\,(\varphi^2(q) - 4q^{1/2}\psi^2(q^2))\\ &= \frac{\eta^2(\tau)}{\eta^4(2\tau)}\,\varphi^2(-q^{1/2}) = \frac{\eta^4(\tau/2)}{\eta^4(2\tau)}.\end{aligned}$$

The result for u_5 may be proved by 5-dissecting the series for the product $\prod_{j=1}^{\infty}(1-q^j)$. See [4, pp. 161–163] or [23] for the details. For different proofs using modular forms, see [19, (7.2)] or [24].

Each result for w_n can be obtained from the corresponding result for u_n by replacing $q^{1/n}$ with $\omega q^{1/n}$, where ω is any nth root of unity, and multiplying the resulting n identities together. Here $n = 2$, 3, 4 or 5. The details in the case $n = 5$ are described in [4, p. 164], [23] and [28], and the proofs in the other cases are similar. ■

The identities in Theorem 3.1 hold because of properties of Hauptmoduls associated with groups of genus 0. For more information, the reader is referred to [13] where many examples of such identities are given.

The u_n and w_n satisfy the following transformation formulas.

THEOREM 3.2.

$$\begin{aligned} u_2(e^{-2\pi/3t}) &= \frac{\frac{1}{3} - u_2(e^{-2\pi t})}{1 + u_2(e^{-2\pi t})}, & w_2(e^{-\pi/3t}) &= \frac{\frac{1}{9} - w_2(e^{-2\pi t})}{1 - w_2(e^{-2\pi t})},\\ u_3(e^{-\pi/t}) &= \frac{\frac{1}{2} - u_3(e^{-2\pi t})}{1 + u_3(e^{-2\pi t})}, & w_3(e^{-\pi/3t}) &= \frac{\frac{1}{8} - w_3(e^{-2\pi t})}{1 + w_3(e^{-2\pi t})},\\ u_4(e^{-2\pi/t}) &= \frac{\frac{1}{2} - u_4(e^{-2\pi t})}{1 + 2u_4(e^{-2\pi t})}, & w_4(e^{-\pi/2t}) &= \frac{1}{16} - w_4(e^{-2\pi t}),\\ u_5(e^{-2\pi/t}) &= \frac{\gamma - u_5(e^{-2\pi t})}{1 + \gamma u_5(e^{-2\pi t})}, & w_5(e^{-2\pi/5t}) &= \frac{\gamma^5 - w_5(e^{-2\pi t})}{1 + \gamma^5 w_5(e^{-2\pi t})}.\end{aligned}$$

Proof. Let $q_1 = \exp(2\pi i\tau)$ and $q_2 = \exp(-2\pi i/3\tau)$. By Theorem 3.1 and the modular transformation (2.1), we have

$$\frac{1}{u_2(q_1)} - 2 - 3u_2(q_1) = \frac{\eta^2(\tau/2)\eta^2(3\tau/2)}{\eta^2(2\tau)\eta^2(6\tau)} = 16\,\frac{\eta^2(-2/\tau)\eta^2(-2/3\tau)}{\eta^2(-1/2\tau)\eta^2(-1/6\tau)}$$
$$= 16\left(\frac{1}{u_2(q_2)} - 2 - 3u_2(q_2)\right)^{-1}.$$

This simplifies to

$$(3.2)\qquad (3u_2(q_1)u_2(q_2) + 3u_2(q_1) + 3u_2(q_2) - 1)$$
$$\times\,(3u_2(q_1)u_2(q_2) - u_2(q_1) - u_2(q_2) - 1) = 0.$$

We claim that the first factor is zero. To see this, take $\tau = i/\sqrt{3}$ and observe that $q_1 = q_2 = \exp(-2\pi/\sqrt{3})$, and hence $u_2(q_1) = u_2(q_2)$. Now

$$u_2(q) = q^{1/2}(1 - 2q + 3q^2 - 4q^3 + 7q^4 + \cdots),$$

and taking just the first term gives

$$u_2(\exp(-2\pi/\sqrt{3})) \approx \exp(-\pi/\sqrt{3}) \approx 0.16.$$

More accurate values can be obtained by using more terms, but this value is good enough for our purpose. The first factor in (3.2) reduces to $3u_2^2+6u_2-1$, which has roots $u_2 = -1 \pm 2/\sqrt{3}$. The second factor in (3.2) reduces to $3u_2^2 - 2u_2 - 1$, which has roots $u_2 = 1,\ -1/3$. The only root that is near 0.16 is $-1 + 2/\sqrt{3}$, hence we select the first factor in (3.2). This proves the claim. It follows that

$$u_2(q_1) = \frac{\frac{1}{3} - u_2(q_2)}{1 + u_2(q_2)},$$

and this completes the proof of the first result.

All of the other results, except for the one that involves w_4, can be deduced in the same way from the corresponding results in Theorem 3.1; we omit the details.

We will now prove the result for w_4. Let

$$f(\tau) = w_4(e^{2\pi i\tau}) + w_4(e^{-i\pi/2\tau}).$$

By (2.1), (2.3) and (2.7), we find

$$f(\tau) = \frac{\eta^8(\tau)\eta^{16}(4\tau)}{\eta^{24}(2\tau)} + \frac{\eta^8(-1/4\tau)\eta^{16}(-1/\tau)}{\eta^{24}(-1/2\tau)}$$
$$= \frac{\eta^8(\tau)\eta^{16}(4\tau)}{\eta^{24}(2\tau)} + \frac{1}{16}\,\frac{\eta^8(4\tau)\eta^{16}(\tau)}{\eta^{24}(2\tau)}$$
$$= \frac{1}{16}\,\frac{\eta^8(\tau)\eta^8(4\tau)}{\eta^{20}(2\tau)}\left(16\,\frac{\eta^8(4\tau)}{\eta^4(2\tau)} + \frac{\eta^8(\tau)}{\eta^4(2\tau)}\right)$$
$$= \frac{1}{16\varphi^4(q)}\,(16q\psi^4(q^2) + \varphi^4(-q)) = \frac{1}{16},$$

and the claimed result follows. ∎

Remark 3.3. There is another transformation for u_4:

$$u_4^2(e^{-\pi/t}) = \frac{\frac{1}{4} - u_4^2(e^{-2\pi t})}{1 + 4u_4^2(e^{-2\pi t})},$$

but we will not need this.

The result for w_3 in the next theorem was given in [14], and the result for w_5 was given by Ramanujan in the lost notebook [1, p. 91].

Theorem 3.4. *Let N be a positive integer and put $q_1 = \exp(-2\pi\sqrt{t/N})$ and $q_2 = \exp(-2\pi/\sqrt{Nt})$. Then*

$$\begin{aligned}
(1 - w_2(q_1))(1 - w_2(q_2)) &= \frac{8}{9} && \text{for } N = 6,\\
(1 + w_3(q_1))(1 + w_3(q_2)) &= \frac{9}{8} && \text{for } N = 6,\\
w_4(q_1) + w_4(q_2) &= \frac{1}{16} && \text{for } N = 4,\\
(1 + \gamma^5 w_5(q_1))(1 + \gamma^5 w_5(q_2)) &= 1 + \gamma^{10} && \text{for } N = 5.
\end{aligned}$$

Proof. These are just restatements of the results for w_n in Theorem 3.2. ∎

Theorem 3.5. *For $n = 2, 3, 4$ or 5, let $v_n = v_n(q)$ and $w_n = w_n(q)$. The following modular equations hold:*

$$\begin{aligned}
v_2 &= \frac{1 - \left(\frac{1-9w_2}{1-w_2}\right)^{1/2}}{3 + \left(\frac{1-9w_2}{1-w_2}\right)^{1/2}}, & w_2 &= v_2\,\frac{1 - v_2}{1 + 3v_2},\\
v_3 &= \frac{1 - \left(\frac{1-8w_3}{1+w_3}\right)^{1/3}}{2 + \left(\frac{1-8w_3}{1+w_3}\right)^{1/3}}, & w_3 &= v_3\,\frac{1 - v_3 + v_3^2}{1 + 2v_3 + 4v_3^2},\\
2v_4 &= \frac{1 - (1 - 16w_4)^{1/4}}{1 + (1 - 16w_4)^{1/4}}, & w_4 &= v_4\,\frac{1 + 4v_4^2}{(1 + 2v_4)^4},\\
v_5 &= \frac{\gamma - \left(\frac{\gamma^5 - w_5}{1+\gamma^5 w_5}\right)^{1/5}}{1 + \gamma\left(\frac{\gamma^5 - w_5}{1+\gamma^5 w_5}\right)^{1/5}}, & w_5 &= v_5\,\frac{1 - 2v_5 + 4v_5^2 - 3v_5^3 + v_5^4}{1 + 3v_5 + 4v_5^2 + 2v_5^3 + v_5^4}.
\end{aligned}$$

Proof. Consider the two identities in Theorem 3.2 that involve u_2 and w_2. Replacing t with $2t$ in the first identity and combining with the second identity gives

$$\left(\frac{\frac{1}{3} - u_2(e^{-4\pi t})}{1 + u_2(e^{-4\pi t})}\right)^2 = \frac{\frac{1}{9} - u_2^2(e^{-2\pi t})}{1 - u_2^2(e^{-2\pi t})},$$

that is,

$$\left(\frac{\frac{1}{3}-v_2}{1+v_2}\right)^2=\frac{\frac{1}{9}-w_2}{1-w_2}.$$

Now solve for v_2 or w_2.

The other results may be proved similarly. ∎

The formula in Theorem 3.5, expressing w_5 as a rational function of v_5, is in Ramanujan's first letter to Hardy [6, p. 29]. The earliest proof known to the author is due to Rogers [25]. The results involving v_3 and w_3 must also be regarded as being known to Ramanujan, as they are trivial consequences of parts (i) and (ii) of Entry 1 in Chapter 20 of his second notebook [2, p. 345]. For additional information, see [1, pp. 95–98].

4. The functions z_n, A_n and M_n. For $n = 2, 3, 4$ or 5, define z_n, k_n, A_n and the multiplier M_n by

$$z_n=z_n(q)=nq\,\frac{d}{dq}\log u_n=q\,\frac{d}{dq}\log w_n;$$
$$k_n=\begin{cases}9 & \text{if } n=2,\\ 8 & \text{if } n=3,\\ 16 & \text{if } n=4,\\ 1/\gamma^5 & \text{if } n=5;\end{cases}$$
$$A_n=A_n(q)=\frac{z_n}{1-k_nu_n^n};$$
$$M_n=M_n(q)=\frac{A_n(q)}{A_n(q^n)}.$$

The reason for the choice of k_n and A_n in these definitions will become clear in Theorem 4.5 and its proof, namely, each function A_n has a particularly simple transformation property.

Most of the results in the next theorem are classical. The results for z_2 and z_4 imply the well-known formulas for the number of representations of an integer by the quadratic forms $x_1^2+x_2^2+3x_3^2+3x_4^2$ and $x_1^2+x_2^2+x_3^2+x_4^2$, respectively. The result for z_5 is equivalent to part (v) of Entry 9 in Chapter 19 of Ramanujan's second notebook [2, p. 258], and the result for z_3 is in Fine's book [20, (32.65)].

Theorem 4.1.

$$z_2=\frac{\eta^4(\tau)\eta^4(3\tau)}{\eta^2(2\tau)\eta^2(6\tau)},\qquad z_3=\frac{\eta^3(\tau)\eta^3(2\tau)}{\eta(3\tau)\eta(6\tau)},\qquad z_4=\frac{\eta^8(\tau)}{\eta^4(2\tau)},\qquad z_5=\frac{\eta^5(\tau)}{\eta(5\tau)}.$$

Proof. Recall the identity [29, p. 451, Ex. 5]

$$\frac{\sigma(a+b)\sigma(a-b)}{\sigma^2(a)\sigma^2(b)}=\wp(b)-\wp(a),$$

where $\wp$ and σ are the Weierstrass elliptic and sigma functions. Explicitly, this is

$$(4.1)\qquad (x-z)\prod_{j=1}^{\infty}\frac{(1-xzq^{j-1})(1-q^jxz^{-1})(1-q^jx^{-1}z)(1-q^jx^{-1}z^{-1})(1-q^j)^4}{(1-xq^{j-1})^2(1-zq^{j-1})^2(1-q^jx^{-1})^2(1-q^jz^{-1})^2}$$
$$=\frac{x}{(1-x)^2}-\frac{z}{(1-z)^2}+\sum_{j=1}^{\infty}\frac{jq^j}{1-q^j}\,(x^j+x^{-j}-z^j-z^{-j}),$$

provided $|q|<|x|,\ |z|<|q|^{-1}$. The results in Theorem 4.1 follow by taking $(x,z)=(e^{i\pi/3},-1)$, $(e^{i\pi/3},e^{2\pi i/3})$, $(i,-1)$ and $(e^{2\pi i/5},e^{4\pi i/5})$, respectively, and simplifying the resulting series and products. Full details for the last case are given in [18]; the details for the other cases are similar. ∎

The next result shows that $A_2(q)$ and $A_3(q)$ are equal.

THEOREM 4.2. *With $A_2(q)$ and $A_3(q)$ as defined above,*

$$A_2(q)=A_3(q)=\frac{\eta^7(2\tau)\eta^7(3\tau)}{\eta^5(\tau)\eta^5(6\tau)}.$$

Proof. Replace q with $-q$ in (2.9) and multiply the resulting identity by (2.9), to get

$$q\psi^4(q^2)-9q^3\psi^4(q^6)=\frac{\eta^5(2\tau)\eta^3(12\tau)}{\eta(4\tau)\eta^3(6\tau)}.$$

Therefore,

$$(4.2)\qquad 1-9u_2^2=1-9\,\frac{\eta^4(\tau)\eta^8(6\tau)}{\eta^8(2\tau)\eta^4(3\tau)}$$
$$=\frac{\eta^4(\tau)}{\eta^8(2\tau)}\,q^{1/2}(\psi^4(q)-9q\psi^4(q^3))=\frac{\eta^9(\tau)\eta^3(6\tau)}{\eta^9(2\tau)\eta^3(3\tau)}.$$

By [2, p. 347] and (2.3), we have

$$(4.3)\qquad 1-8u_3^3=1-8\,\frac{\eta^3(\tau)\eta^9(6\tau)}{\eta^3(2\tau)\eta^9(3\tau)}=\frac{\varphi^4(-q)}{\varphi^4(-q^3)}=\frac{\eta^8(\tau)\eta^4(6\tau)}{\eta^4(2\tau)\eta^8(3\tau)}.$$

Now use (4.2) and (4.3) in the definitions of A_2 and A_3 and use Theorem 4.1 to complete the proof. ∎

The next result expresses the multipliers M_n as rational functions of v_n.

THEOREM 4.3. *For $n=2$, 3, 4 or 5, let $v_n=v_n(q)$ and $M_n=M_n(q)$. Then*

$$M_2=\frac{(1+v_2)(1+3v_2)}{1-v_2},$$
$$M_3=\frac{(1+v_3)^2(1+2v_3+4v_3^2)}{1-v_3+v_3^2},$$

$$M_4 = (1+2v_4)^4,$$
$$M_5 = \frac{(1+\gamma v_5)^4(\gamma^2+v_5+v_5^2)}{\gamma^2(1-v_5+\gamma^2 v_5^2)}.$$

Proof. Let us prove the result for M_2. If we start with the definition of M_2 and apply Theorem 4.1, we find that

$$\begin{aligned} M_2 &= \frac{A_2(q)}{A_2(q^2)} = \frac{z_2(q)}{z_2(q^2)} \cdot \frac{1-9v_2^2}{1-9u_2^2} \\ &= \frac{\eta^4(\tau)\eta^4(3\tau)}{\eta^2(2\tau)\eta^2(6\tau)} \cdot \frac{\eta^2(4\tau)\eta^2(12\tau)}{\eta^4(2\tau)\eta^4(6\tau)} \cdot \frac{1-9v_2^2}{1-9u_2^2} \\ &= \frac{\eta^6(\tau)\eta^6(3\tau)}{\eta^6(2\tau)\eta^6(6\tau)} \cdot \frac{\eta^2(4\tau)\eta^2(12\tau)}{\eta^2(\tau)\eta^2(3\tau)} \cdot \frac{1-9v_2^2}{1-9u_2^2}. \end{aligned}$$

Apply Theorem 3.1 to this, to get

$$\begin{aligned} M_2 &= \frac{\frac{1}{u_2^2} - 10 + 9u_2^2}{\frac{1}{v_2} - 2 - 3v_2} \cdot \frac{1-9v_2^2}{1-9u_2^2} = \frac{(1-u_2^2)v_2(1+3v_2)}{u_2^2(1+v_2)} \\ &= \frac{(1-w_2)v_2(1+3v_2)}{w_2(1+v_2)}. \end{aligned}$$

Now use Theorem 3.5 to express w_2 in terms of v_2. This completes the proof of the result for M_2.

The results for M_3 and M_5 can be proved by exactly the same method, and the details are given in [14, (4.15)] and [11, (3.12)], respectively.

It remains to prove the result for M_4. By the definition of M_4 and Theorem 4.1, we have

$$\begin{aligned} M_4 &= \frac{A_4(q)}{A_4(q^4)} = \frac{z_4(q)}{z_4(q^4)} \cdot \frac{1-16v_4^4}{1-16u_4^4} \\ &= \frac{\eta^8(\tau)}{\eta^4(2\tau)} \cdot \frac{\eta^4(8\tau)}{\eta^8(4\tau)} \cdot \frac{1-16v_4^4}{1-16u_4^4} \\ &= \frac{\eta^4(8\tau)}{\eta^4(2\tau)} \cdot \frac{\eta^{12}(\tau)}{\eta^{12}(2\tau)} \cdot \frac{\eta^{12}(2\tau)}{\eta^4(\tau)\eta^8(4\tau)} \cdot \frac{1-16v_4^4}{1-16u_4^4}. \end{aligned}$$

Apply Theorem 3.1 to this, and making use of the definitions of u_4 and w_4, we obtain

$$M_4 = \frac{\frac{1}{u_4^2} - 16u_4^2}{u_4^2(\frac{1}{v_4} - 4v_4)} \cdot \frac{1-16v_4^4}{1-16u_4^4} = \frac{v_4}{w_4}(1+4v_4^2).$$

Now use Theorem 3.5 to express w_4 in terms of v_4. This completes the proof. ■

THEOREM 4.4. *For $n = 2$, 3, 4 or 5, let $v_n = v_n(q)$ and $M_n = M_n(q)$. Then*

$$\frac{1}{M_n A_n(q^n)}\, q\, \frac{d}{dq} M_n = \frac{v_n}{M_n}\,(1 - k_n v_n^n)\,\frac{dM_n}{dv_n}.$$

Proof. By the chain rule and the definitions of u_n, v_n, z_n and A_n, we have

$$\begin{aligned} q\,\frac{d}{dq} M_n &= \frac{dM_n}{dv_n}\, q\,\frac{d}{dq} u(q^n) = \frac{dM_n}{dv_n}\, z_n(q^n) u_n(q^n) \\ &= \frac{dM_n}{dv_n}\, A_n(q^n)(1 - k_n v_n^n) v_n. \end{aligned}$$

The result follows. ∎

Observe that the right hand side of the identity in Theorem 4.4 may be expressed as a rational function of v_n, by Theorem 4.3. This fact will be used in Section 7 to construct iterations for $1/\pi$.

The last result in this section is

THEOREM 4.5. *Let*

$$N = \begin{cases} 6 & \textit{if } n = 2 \textit{ or } 3, \\ 4 & \textit{if } n = 4, \\ 5 & \textit{if } n = 5. \end{cases}$$

Then, with $A_n = A_n(q)$ and $\widetilde{A_n} = q\frac{d}{dq} A_n(q)$, we have for $n = 2$, 3, 4 and 5,

$$tA_n(e^{-2\pi\sqrt{t/N}}) = A_n(e^{-2\pi/\sqrt{Nt}}) \tag{4.4}$$

and

$$\sqrt{t}\,\frac{\widetilde{A_n}}{A_n}\,(e^{-2\pi\sqrt{t/N}}) + \frac{1}{\sqrt{t}}\,\frac{\widetilde{A_n}}{A_n}\,(e^{-2\pi/\sqrt{Nt}}) = \frac{\sqrt{N}}{\pi}. \tag{4.5}$$

Proof. We prove the result for $n = 2$. The proofs in the other cases are similar. Write $q_1 = \exp(-2\pi\sqrt{t/N})$ and $q_2 = \exp(-2\pi/\sqrt{Nt})$. Apply d/dt to the first result in Theorem 3.4 and apply the definition of z_n to get

$$tz_2(q_1)w_2(q_1)(1 - w_2(q_2)) = z_2(q_2)w_2(q_2)(1 - w_2(q_1)),$$

that is,

$$tz_2(q_1)\,\frac{w_2(q_1)}{1 - w_2(q_1)} = z_2(q_2)\,\frac{w_2(q_2)}{1 - w_2(q_2)}. \tag{4.6}$$

From Theorem 3.2, we deduce

$$\frac{w_2(q_1)}{1 - w_2(q_1)} = \frac{1}{8}\,(1 - 9w_2(q_2)) \quad \text{and} \quad \frac{w_2(q_2)}{1 - w_2(q_2)} = \frac{1}{8}\,(1 - 9w_2(q_1)). \tag{4.7}$$

Substitute (4.7) into (4.6) to get

$$\frac{tz_2(q_1)}{1-9w_2(q_1)} = \frac{z_2(q_2)}{1-9w_2(q_2)},$$

and this proves (4.4) in the case $n = 2$.

The identity (4.5) follows from (4.4) by taking logarithms and differentiating with respect to t. ∎

5. Series. For $n = 2$, 3, 4 or 5, define the weight one modular form φ_n by

$$\varphi_n = \varphi_n(q) = \left(\frac{z_n x_n}{u_n^n}\right)^{1/2}.$$

Infinite products for φ_n may be written down using the definitions for x_n and u_n, (2.3) and the results in Theorem 4.1; we find

$$\varphi_2 = \frac{\eta^6(2\tau)\eta(3\tau)}{\eta^3(\tau)\eta^2(6\tau)} = \frac{\psi^3(q)}{\psi(q^3)}, \tag{5.1}$$

$$\varphi_3 = \frac{\eta(2\tau)\eta^6(3\tau)}{\eta^2(\tau)\eta^3(6\tau)} = \frac{\varphi^3(-q^3)}{\varphi(-q)}, \tag{5.2}$$

$$\varphi_4 = \frac{\eta^{22}(2\tau)}{\eta^{12}(\tau)\eta^8(4\tau)} = \frac{\varphi^4(q)}{\varphi^2(-q)}, \tag{5.3}$$

$$\begin{aligned} \varphi_5 &= \left\{\frac{\eta^5(5\tau)}{\eta(\tau)} \cdot \frac{1}{q} \prod_{j=1}^{\infty} \frac{(1-q^{5j-3})^5(1-q^{5j-2})^5}{(1-q^{5j-4})^5(1-q^{5j-1})^5}\right\}^{1/2} \\ &= \prod_{j=1}^{\infty} \frac{(1-q^j)^2}{(1-q^{5j-4})^5(1-q^{5j-1})^5}. \end{aligned} \tag{5.4}$$

The next result gives differential equations for φ_n. For more information about the differential equations (5.5), (5.6) and (5.8) that occur below, see the work of H. Verrill [27]. The differential equation (5.8) has been studied in detail by F. Beukers [7].

Theorem 5.1.

$$\frac{d}{dw_2}\left(w_2(1-w_2)(1-9w_2)\frac{d\varphi_2}{dw_2}\right) = 3(1-3w_2)\varphi_2, \tag{5.5}$$

$$\frac{d}{dw_3}\left(w_3(1+w_3)(1-8w_3)\frac{d\varphi_3}{dw_3}\right) = 2(1+4w_3)\varphi_3, \tag{5.6}$$

$$\frac{d}{dw_4}\left(w_4(1-16w_4)^2\frac{d\varphi_4}{dw_4}\right) = 4(3-64w_4)\varphi_4, \tag{5.7}$$

$$\frac{d}{dw_5}\left(w_5(1-11w_5-w_5^2)\frac{d\varphi_5}{dw_5}\right) = (3+w_5)\varphi_5. \tag{5.8}$$

We shall prove the results in Theorem 5.1 one at a time. The proofs follow the method in [14], and each of (5.5)–(5.8) is derived from a known differential equation by making a change of variable.

Proof of (5.5). We begin by noting that from the definitions of φ_2 and w_2 and (2.3), we have

$$\varphi_2 = \frac{\psi^3(q)}{\psi(q^3)} \quad \text{and} \quad w_2 = q\,\frac{\psi^4(q^3)}{\psi^4(q)}. \tag{5.9}$$

We claim that

$$a(q) = (1+3w_2)\varphi_2 \quad \text{and} \quad \frac{c^3(q)}{a^3(q)} = \frac{27w_2(1-w_2)^2}{(1+3w_2)^3}. \tag{5.10}$$

The first part follows from lines 2 and 4 of Entry 3(i) in Chapter 21 of Ramanujan's second notebook [2, p. 460] and using (2.11). To prove the second part, replace q with $-q$ in (2.8) and multiply the resulting identity by (2.8), to get

$$q\psi^4(q^2) - q^3\psi^4(q^6) = \frac{\eta^3(4\tau)\eta^5(6\tau)}{\eta^3(2\tau)\eta(12\tau)}. \tag{5.11}$$

Therefore, applying (5.10), (5.9), (2.3), (5.11) and (2.10), we obtain

$$\begin{aligned}
\frac{w_2(1-w_2)^2}{(1+3w_2)^3} &= \left(\frac{\varphi_2(q)}{a(q)}\right)^3 w_2(1-w_2)^2 \\
&= \frac{1}{a^3(q)}\left(\frac{\psi^3(q)}{\psi(q^3)}\right)^3 q\,\frac{\psi^4(q^3)}{\psi^4(q)}\left(1-q\,\frac{\psi^4(q^3)}{\psi^4(q)}\right)^2 \\
&= \frac{1}{a^3(q)}\,\frac{\psi(q^3)}{\psi^3(q)}\,(q^{1/2}\psi^4(q) - q^{3/2}\psi^4(q^3))^2 \\
&= \frac{1}{a^3(q)}\,\frac{\eta^3(\tau)\eta^2(6\tau)}{\eta(3\tau)\eta^6(2\tau)}\left(\frac{\eta^3(2\tau)\eta^5(3\tau)}{\eta^3(\tau)\eta(6\tau)}\right)^2 \\
&= \frac{1}{a^3(q)}\,\frac{\eta^9(3\tau)}{\eta^3(\tau)} = \frac{1}{27}\,\frac{c^3(q)}{a^3(q)}.
\end{aligned}$$

This proves the second part of the claim in (5.10).

Now let $\mathbf{z}_3 = a(q)$ and $\mathbf{x}_3 = c^3(q)/a^3(q)$. It is known (see, e.g., [3, p. 106, (4.7)], [5], [9], [16]) that

$$\frac{d}{d\mathbf{x}_3}\left(\mathbf{x}_3(1-\mathbf{x}_3)\,\frac{d\mathbf{z}_3}{d\mathbf{x}_3}\right) = \frac{2\mathbf{z}_3}{9}. \tag{5.12}$$

We re-express (5.12) in terms of φ_2 and w_2. By the chain rule and (5.10), we have

$$\frac{d}{d\mathbf{x}_3} = \frac{dw_2}{d\mathbf{x}_3}\,\frac{d}{dw_2} = \frac{(1+3w_2)^4}{27(1-w_2)(1-9w_2)}\,\frac{d}{dw_2},$$

and by (5.10) again, we obtain

$$\mathbf{x}_3(1-\mathbf{x}_3)\,\frac{d}{d\mathbf{x}_3} = \frac{w_2(1-w_2)(1-9w_2)}{(1+3w_2)^2}\,\frac{d}{dw_2}.$$

Hence (5.12) is equivalent to

$$\frac{(1+3w_2)^4}{27(1-w_2)(1-9w_2)}\,\frac{d}{dw_2}\left(\frac{w_2(1-w_2)(1-9w_2)}{(1+3w_2)^2}\,\frac{d\mathbf{z}_3}{dw_2}\right) = \frac{2\mathbf{z}_3}{9}. \tag{5.13}$$

By (5.10) we have $\mathbf{z}_3 = (1+3w_2)\varphi_2$. Using this in (5.13) and simplifying, we obtain (5.5). ∎

Proof of (5.6). A proof has been given by Chan and Loo [14, (5.2)]. The key [14, Lemma 3.1] is to use

$$a(q) = (1+4w_3)\varphi_3 \quad\text{and}\quad \frac{c^3(q)}{a^3(q)} = \frac{27w_3}{(1+4w_3)^3} \tag{5.14}$$

in place of (5.10). ∎

Proof of (5.7). Let $\mathbf{z}_4 = \varphi^2(q)$ and $\mathbf{x}_4 = 16q\psi^4(q^2)/\varphi^4(q)$. By the infinite products for φ_4 and w_4 and Entries 10 and 11 of Chapter 17 of Ramanujan's second notebook [2, pp. 122–123], we have

$$\varphi_4 = \frac{\mathbf{z}_4}{\sqrt{1-\mathbf{x}_4}} \quad\text{and}\quad w_4 = \frac{\mathbf{x}_4}{16}. \tag{5.15}$$

It is known (see, e.g., [2, p. 120, (9.1)], [16]) that

$$\frac{d}{d\mathbf{x}_4}\left(\mathbf{x}_4(1-\mathbf{x}_4)\,\frac{d\mathbf{z}_4}{d\mathbf{x}_4}\right) = \frac{\mathbf{z}_4}{4}. \tag{5.16}$$

Making the change of variable given by (5.15) in (5.16), we obtain (5.7). ∎

Proof of (5.8). In [17, Theorem 2.8] it was shown that

$$a_5x_5z_5\,\frac{d}{dx_5}\left(a_5x_5\,\frac{dz_5}{dx_5}\right) = \frac{1}{2}\left(a_5x_5\,\frac{dz_5}{dx_5}\right)^2 - \frac{5}{2}\,x_5(2+25x_5)z_5^2, \tag{5.17}$$

where

$$a_5 = (1+22x_5+125x_5^2)^{1/2}.$$

We re-express the differential equation (5.17) in terms of φ_5 and w_5. By [17, Theorem 2.4] we have

$$q\,\frac{dx_5}{dq} = a_5x_5z_5 \quad\text{and}\quad q\,\frac{dw_5}{dq} = w_5z_5.$$

It follows that both x_5 and w_5 are increasing functions of q for $-1<q<1$, and therefore by the chain rule we have

$$a_5x_5\,\frac{d}{dx_5} = a_5x_5\left(q\,\frac{dw_5}{dq}\right)\Big/\left(q\,\frac{dx_5}{dq}\right)\frac{d}{dw_5} = w_5\,\frac{d}{dw_5}.$$

Hence (5.17) becomes

$$w_5 z_5 \frac{d}{dw_5}\left(w_5 \frac{dz_5}{dw_5}\right) = \frac{1}{2}\left(w_5 \frac{dz_5}{dw_5}\right)^2 - \frac{5}{2} x_5(2+25x_5)z_5^2. \tag{5.18}$$

Now use the definition of φ_5 and Theorem 3.1 to express z_5 in terms of φ_5 and w_5, i.e.,

$$z_5 = \frac{w_5}{x_5}\varphi_5^2 = (1-11w_5-w_5^2)\varphi_5^2. \tag{5.19}$$

Substitute (5.19) into (5.18), and use Theorem 3.1 to express $x_5(2+25x_5)$ as a rational function of w_5. The result simplifies to (5.8). ∎

THEOREM 5.2. *For $n = 2$, 3, 4 or 5 and $\varphi_n = \varphi_n(q)$ and $w_n = w_n(q)$, we have the series expansions*

$$\varphi_n = \sum_{k=0}^{\infty} c_n(k) w_n^k, \tag{5.20}$$

valid for

$$|w_2| < \frac{1}{9}, \qquad |w_3| < \frac{1}{8}, \qquad |w_4| < \frac{1}{16}, \qquad |w_5| < \gamma^5 \approx 0.09,$$

where the coefficients $c_n(k)$ satisfy the recurrence relations

$$\begin{aligned}
(k+1)^2 c_2(k+1) &= (10k^2+10k+3)c_2(k) - 9k^2 c_2(k-1),\\
(k+1)^2 c_3(k+1) &= (7k^2+7k+2)c_3(k) + 8k^2 c_3(k-1),\\
(k+1)^2 c_4(k+1) &= (32k^2+32k+12)c_4(k) - 256k^2 c_4(k-1),\\
(k+1)^2 c_5(k+1) &= (11k^2+11k+3)c_5(k) + k^2 c_5(k-1).
\end{aligned}$$

The first few terms in each sequence, together with the reference to Sloane's On-line Encyclopedia of Integer Sequences [26], *are given in Table* 1.

Table 1. First few values of $c_n(k)$

n	$c_n(0)$	$c_n(1)$	$c_n(2)$	$c_n(3)$	Sloane id.
2	1	3	15	93	A002893
3	1	2	10	56	A000172
4	1	12	164	2352	N/A
5	1	3	19	147	A005258

Proof. The existence of series solutions in the forms given by (5.20), and the radii of convergence of the series, follow from the standard theory of linear differential equations. The recurrence relations follow by substituting the series (5.20) into the differential equations in Theorem 5.1 and comparing coefficients. The values of $c_n(0)$ and $c_n(1)$ in Table 1 may be computed by expanding both sides of (5.20) in powers of q and comparing the constant term and the coefficient of q. Further values of $c_n(k)$ can then be computed using the recurrence relations. ∎

The recurrence relations in Theorem 5.2 have the following explicit solutions in terms of sums of binomial coefficients.

THEOREM 5.3. *The coefficients $c_n(k)$ are given by*

$$c_2(k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{2j}{j}, \qquad c_3(k) = \sum_{j=0}^{k} \binom{k}{j}^3,$$

$$c_4(k) = \sum_{j=0}^{k} \binom{2j}{j}^2 \binom{2k-2j}{k-j} 2^{2k-2j}, \qquad c_5(k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{j+k}{j}.$$

Proof. The results for $c_2(k)$, $c_3(k)$ and $c_5(k)$ are well-known; see [26] for references. The result for $c_4(k)$ can be deduced from (5.15) and the result

$$\mathbf{z}_4 = {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \mathbf{x}_4\right).$$

Thus,

$$\varphi_4 = (1-16w_4)^{-1/2} \, {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; 16w_4\right).$$

Now expand in powers of w_4 and extract the coefficient of w_4^n. ∎

THEOREM 5.4. *For $k = 2$, 3, 4 or 5, define*

$$C_n(k) = \sum_{j=0}^{k} c_n(j) c_n(k-j).$$

Then, with $A_n = A_n(q)$, $\widetilde{A_n} = q\frac{d}{dq}A_n(q)$ and $w_n = w_n(q)$, we have

$$\frac{\widetilde{A_2}}{A_2} = (1-w_2)(1-9w_2) \sum_{k=0}^{\infty} C_2(k) \left(k - \frac{w_2}{1-w_2}\right) w_2^k,$$

$$\frac{\widetilde{A_3}}{A_3} = (1+w_3)(1-8w_3) \sum_{k=0}^{\infty} C_3(k) \left(k + \frac{w_3}{1+w_3}\right) w_3^k,$$

$$\frac{\widetilde{A_4}}{A_4} = (1-16w_4)^2 \sum_{k=0}^{\infty} C_4(k) \left(k - \frac{16w_4}{1-16w_4}\right) w_4^k,$$

$$\frac{\widetilde{A_5}}{A_5} = (1-11w_5-w_5^2) \sum_{k=0}^{\infty} C_5(k) \left(k + \frac{\gamma^5 w_5}{1+\gamma^5 w_5}\right) w_5^k.$$

The series converge for

$$|w_2| < \frac{1}{9}, \qquad |w_3| < \frac{1}{8}, \qquad |w_4| < \frac{1}{16}, \qquad |w_5| < \gamma^5 \approx 0.09.$$

Proof. By the chain rule and the definitions of z_2 and A_2, we have

$$\frac{1}{A_2}\, q\, \frac{dA_2}{dq} = \frac{1}{A_2}\, q\, \frac{dw_2}{dq}\, \frac{dA_2}{dw_2} = \frac{z_2 w_2}{A_2}\, \frac{dA_2}{dw_2} = (1-9w_2)w_2\, \frac{dA_2}{dw_2}. \tag{5.21}$$

By the definitions of A_2 and φ_2, followed by Theorem 3.1, we have

$$\begin{aligned} A_2 &= \frac{z_2}{1-k_2w_2} = \frac{w_2}{x_2(1-k_2w_2)}\, \varphi_2^2 \\ &= \frac{1-10w_2+9w_2^2}{1-9w_2}\, \varphi_2^2 = (1-w_2)\varphi_2^2 \\ &= (1-w_2)\sum_{k=0}^{\infty} C_2(k) w_2^k. \end{aligned} \tag{5.22}$$

Substituting (5.22) into the right hand side of (5.21) we obtain the first result.

The other results may be obtained similarly. ∎

The next goal is to find values of q which yield explicit values for w_n and $\widetilde{A_n}/A_n$ in Theorem 5.4. These will imply series for $1/\pi$.

THEOREM 5.5. *With $A_n = A_n(q)$, $\widetilde{A_n} = q\frac{d}{dq}A_n(q)$ and $w_n = w_n(q)$, we have*

$$\begin{aligned} \frac{\widetilde{A_2}}{A_2}\,(e^{-2\pi/\sqrt{6}}) &= \frac{\sqrt{6}}{2\pi}, & w_2(e^{-2\pi/\sqrt{6}}) &= \frac{1}{3}\,(3-\sqrt{8}), \\ \frac{\widetilde{A_3}}{A_3}\,(e^{-2\pi/\sqrt{6}}) &= \frac{\sqrt{6}}{2\pi}, & w_3(e^{-2\pi/\sqrt{6}}) &= \frac{1}{4}\,(3\sqrt{2}-4), \\ \frac{\widetilde{A_4}}{A_4}\,(e^{-\pi}) &= \frac{1}{\pi}, & w_4(e^{-\pi}) &= \frac{1}{32}, \\ \frac{\widetilde{A_5}}{A_5}\,(e^{-2\pi/\sqrt{5}}) &= \frac{\sqrt{5}}{2\pi}, & w_5(e^{-2\pi/\sqrt{5}}) &= \frac{1}{\gamma^5}\,(\sqrt{1+\gamma^{10}}-1). \end{aligned}$$

Proof. The values in the left column follow by taking $t = 1$ in (4.5). The values in the right column follow by taking $t = 1$ in Theorem 3.4 and solving the resulting quadratic equation. The appropriate root can be determined by using the approximation $w_n(q) \approx q$. ∎

If the values in Theorem 5.5 are substituted into the series in Theorem 5.4, the results are the series for $1/\pi$ given by (1.1)–(1.4) in the introduction. In each case, the value of w_n in Theorem 5.5 is approximately one half of the radius of convergence, so the series yields approximately one binary digit (or about 0.3 decimal places) per term.

The coefficients $C_n(k)$ may be computed efficiently using third order recurrence relations. For example, $C_4(k)$ satisfies the recurrence relation

$$\begin{aligned}(k+1)^3 C_4(k+1) &= 8(3+10k+12k^2+6k^3)C_4(k)\\ &\quad -128(1+4k+6k^2+6k^3)C_4(k-1)+4096k^3C_4(k-2),\end{aligned}$$

where

$$C_4(0)=1, \qquad C_4(1)=24, \qquad C_4(2)=472.$$

We point out that taking only the $k=0$ term in (1.3) gives the (really bad!) approximation $\pi=-4$. Despite this poor start, the series then proceeds to converge at approximately one binary digit per term.

6. A divergent series. The functions φ_2 and z_2 are modular forms of weights 1 and 2, respectively, on $\Gamma_0(6)_{+3}$, and likewise, φ_3 and z_3 are modular forms of weights 1 and 2, respectively, on $\Gamma_0(6)_{+2}$. It remains to investigate the space $\Gamma_0(6)_{+6}$, and that is the topic of this section. There are some fundamental differences for the space $\Gamma_0(6)_{+6}$. For example, there is no analogue of the function u_n, and the resulting series analogue of Theorem 5.4 with $q=e^{-2\pi/\sqrt{6}}$ leads to a series for $1/\pi$ that does not converge. A sketch of the theory is as follows.

Let

$$w_6=\frac{\eta(2\tau)\eta^5(6\tau)}{\eta^5(\tau)\eta(3\tau)}, \qquad x_6=\frac{\eta(\tau)^{12}\eta^{12}(6\tau)}{\eta^{12}(2\tau)\eta^{12}(3\tau)},$$
$$z_6=q\frac{d}{dq}\log w_6, \qquad A_6=z_6, \qquad \varphi_6=\left(\frac{z_6x_6}{w_6}\right)^{1/2}.$$

The analogues of Theorems 3.1 and 3.2 are

$$\frac{1}{w_6}+17+72w_6=\frac{1}{x_6} \quad\text{and}\quad w_6(e^{-2\pi t})w_6(e^{-\pi/3t})=\frac{1}{72}, \tag{6.1}$$

and the analogues of Theorem 4.1 and (5.1) and (5.2) are

$$z_6=\frac{\eta^7(2\tau)\eta^7(3\tau)}{\eta^5(\tau)\eta^5(6\tau)}=A_2=A_3=A_6 \quad\text{and}\quad \varphi_6=\frac{\eta^6(\tau)\eta(6\tau)}{\eta^3(2\tau)\eta^2(3\tau)}.$$

In place of (5.10) and (5.14) we have

$$a(q)=(1+12w_6)\varphi_6 \quad\text{and}\quad \frac{c^3(q)}{a^3(q)}=\frac{27w_6(1+8w_6)^2}{(1+12w_6)^3},$$

and these may be used to derive the differential equation

$$\frac{d}{dw_6}\left(w_6(1+8w_6)(1+9w_6)\frac{d\varphi_6}{dw_6}\right)+6(1+12w_6)\varphi_6=0.$$

This has the power series solution

$$\varphi_6 = \sum_{k=0}^{\infty} c_6(k) w_6^k,$$

valid for $|w_6| < 1/9$, where the coefficients $c_6(k)$ satisfy the recurrence relation

$$(k+1)^2 c_6(k+1) = -(17k^2 + 17k + 6)c_k - 72k^2 c_{k-1}$$

and are given explicitly by the formula

$$c_6(k) = \sum_{j=0}^{k} \binom{k}{j} (-8)^j \sum_{i=0}^{k-j} \binom{k-j}{i}^3.$$

The sequence $(-1)^k c_6(k)$ is A093388 in Sloane's database [26]. The first few terms are given by

$$c_6(0) = 1, \qquad c_6(1) = -6, \qquad c_6(2) = 42, \qquad c_6(3) = -312.$$

The analysis at the end of the previous section can now be applied. The result is

$$\frac{\widetilde{A_6}}{A_6} = (1+8w_6)(1+9w_6) \sum_{k=0}^{\infty} C_6(k) \left(k + \frac{17w_6 + 144w_6^2}{(1+8w_6)(1+9w_6)} \right) w_6^k, \tag{6.2}$$

provided $|w_6| < 1/9$, and where $C_6(k) = \sum_{j=0}^{k} c_6(j) c_6(k-j)$. Now take $q = e^{-2\pi/\sqrt{6}}$. Since $A_6 = A_2$, we have $\widetilde{A_6}/A_6 = \sqrt{6}/2\pi$. By the second part of (6.1) we find $w_6 = 1/\sqrt{72} \approx 0.118$, but this is outside the interval of convergence. In order to obtain a convergent series for $1/\pi$ from (6.2), a different value of q that yields a smaller value of w_6 will have to be used.

7. Iterations. In this section we use the ideas from [14], that were utilized in [11], to produce four iterations that converge to $1/\pi$. One of these (the case $n = 2$) is new. Another new iteration, based on the Ramanujan–Göllnitz–Gordon continued fraction, will be developed in Section 8.

Throughout this section, for $n = 2$, 3, 4 or 5, let

$$N = \begin{cases} 6 & \text{if } n = 2 \text{ or } 3, \\ 4 & \text{if } n = 4, \\ 5 & \text{if } n = 5. \end{cases}$$

Let $A_n = A_n(q)$, $\widetilde{A_n} = q\frac{d}{dq}A_n(q)$ and put $q = \exp(-2\pi\sqrt{t/N})$, where t is a positive real variable. Define $\kappa_n = \kappa_n(t)$ by

$$\kappa_n(t) = \frac{1}{\pi A_n} - 2\sqrt{\frac{t}{N}}\,\frac{\widetilde{A_n}}{A_n^2}.$$

Iterations for $1/\pi$ can be constructed from the following properties of κ_n.

THEOREM 7.1. *With $M_n = M_n(q)$, $\widetilde{M_n} = q\frac{d}{dq}M_n(q)$ and $q = e^{-2\pi\sqrt{t/N}}$, we have*

$$\kappa_n(t) + t\kappa_n\left(\frac{1}{t}\right) = 0, \tag{7.1}$$

$$\kappa_n(n^2 t) = M_n\kappa_n(t) + 2\sqrt{\frac{t}{N}}\,\frac{\widetilde{M_n}}{M_n A_n(q^n)}, \tag{7.2}$$

and

$$\kappa_n(t) = \frac{1}{\pi} - (b_1 + b_2\sqrt{t})q + O(\sqrt{t}\,q^2) \qquad \text{as } t \to \infty, \tag{7.3}$$

where

$$b_1 = \begin{cases} 5/\pi & \text{if } n = 2 \text{ or } 3, \\ 8/\pi & \text{if } n = 4, \\ (1+5\sqrt{5})/2\pi & \text{if } n = 5, \end{cases}$$

and

$$b_2 = \begin{cases} 10/\sqrt{6} & \text{if } n = 2 \text{ or } 3, \\ 8 & \text{if } n = 4, \\ 1/\sqrt{5}+5 & \text{if } n = 5. \end{cases}$$

Proof. The identity (7.1) follows from (4.5) by dividing by $A_n(e^{-2\pi\sqrt{t/N}})$, applying (4.4) and expressing the result in terms of κ_n.

The identity (7.2) can be obtained by applying logarithmic differentiation to the definition of M_n and expressing the result in terms of κ_n.

Finally, (7.3) follows by computing the first two terms in the q-expansions of $1/A_n$ and $\widetilde{A_n}/A_n^2$. ∎

For $n = 2$, 3, 4 or 5, define sequences $\{k_j\}$ and $\{s_j\}$ by

$$k_j = \kappa_n(n^{2j}), \qquad s_j = u_n(\exp(-2\pi n^j/\sqrt{N})).$$

The asymptotic formula (7.3) implies that k_j converges to $1/\pi$ with order n. A recurrence relation for s_j follows immediately from the results in Theorem 3.5, and a recurrence relation giving k_{j+1} in terms of k_j and s_{j+1} is implied by the functional equation (7.2). We give the full details in the case $n = 2$. By Theorem 3.5 we have

$$s_{j+1} = \frac{1 - \left(\frac{1-9s_j^2}{1-s_j^2}\right)^{1/2}}{3 + \left(\frac{1-9s_j^2}{1-s_j^2}\right)^{1/2}} \tag{7.4}$$

and from Theorem 5.5 we find

$$s_0 = u_2(e^{-2\pi/\sqrt{6}}) = \left(1 - \frac{\sqrt{8}}{3}\right)^{1/2} = \frac{\sqrt{6}-\sqrt{3}}{3}. \tag{7.5}$$

By Theorem 4.3 and the definitions of v_2 and s_j, we have

$$M_2(e^{-2^{j+1}\pi/\sqrt{6}}) = \left.\frac{(1+v_2)(1+3v_2)}{1-v_2}\right|_{q=\exp(-2^{j+1}\pi/\sqrt{6})} = \frac{(1+s_{j+1})(1+3s_{j+1})}{1-s_{j+1}}. \tag{7.6}$$

By Theorems 4.3 and 4.4 we have

$$\begin{aligned}\frac{1}{M_2A_2(q^2)}\,q\,\frac{dM_2}{dq} &= \frac{v_2}{M_2}\,(1-9v_2^2)\,\frac{dM_2}{dv_2}\\ &= \frac{v_2(1-v_2)(1-9v_2^2)}{(1+v_2)(1+3v_2)}\,\frac{d}{dv_2}\left\{\frac{(1+v_2)(1+3v_2)}{1-v_2}\right\}\\ &= \frac{v_2(1-3v_2)(5+6v_2-3v_2^2)}{1-v_2^2},\end{aligned}$$

therefore

$$\left.\frac{\widetilde{M_2}}{M_2A_2(q^2)}\right|_{q=e^{-2^{j+1}\pi/\sqrt{6}}} = \frac{s_{j+1}(1-3s_{j+1})(5+6s_{j+1}-3s_{j+1}^2)}{1-s_{j+1}^2}. \tag{7.7}$$

Taking $t=2^{2j}$ in (7.2) and using (7.6) and (7.7), we obtain the recurrence relation

$$\begin{aligned}k_{j+1} &= \frac{(1+s_{j+1})(1+3s_{j+1})}{1-s_{j+1}}\,k_j\\ &\quad+\frac{2^{j+1}}{\sqrt{6}}\,\frac{s_{j+1}(1-3s_{j+1})(5+6s_{j+1}-3s_{j+1}^2)}{1-s_{j+1}^2}\end{aligned} \tag{7.8}$$

and from (7.1) we deduce

$$k_0 = 0. \tag{7.9}$$

Thus, we have proved

THEOREM 7.2. *Consider the sequences given by the recurrence relations* (7.4) *and* (7.8), *together with the initial conditions in* (7.5) *and* (7.9). *Then* $k_j \to 1/\pi$ *as* $j\to\infty$, *and the convergence is quadratic.*

The details of the cubic iteration that arises in the case $n=3$ were worked out by Chan and Loo in [14]. The quartic iteration for $n=4$ turns out to be equivalent to one given by Chan in [10, Iteration 1.6]. The quintic iteration for $n=5$ was given by Chan, Cooper and Liaw in [11].

8. Another iteration for $1/\pi$.

Let

$$u = u(q) = q^{1/2}\prod_{j=1}^{\infty}\frac{(1-q^{8j-7})(1-q^{8j-1})}{(1-q^{8j-5})(1-q^{8j-3})}$$

and define

$$v = v(q) = u(q^2), \qquad w = w(q) = u^2(q).$$

The function u has an expansion as a continued fraction, called the Ramanujan–Göllnitz–Gordon continued fraction. In this section we outline an iteration for $1/\pi$ that comes from exploiting properties of the Ramanujan–Göllnitz–Gordon continued fraction. We have been unable to find a series like the ones in Theorem 5.4, because we have been unable to find the corresponding weight one modular form.

THEOREM 8.1. *Let $\alpha = \sqrt{2} - 1$. Let $k_0 = 0$ and $s_0 = \frac{1}{\alpha}\sqrt{1 - \sqrt{1 - \alpha^4}}$, and define sequences by*

$$s_{j+1} = \frac{\alpha - \left(\frac{\alpha^2 - s_j^2}{1 - \alpha^2 s_j^2}\right)^{1/2}}{1 + \alpha\left(\frac{\alpha^2 - s_j^2}{1 - \alpha^2 s_j^2}\right)^{1/2}},$$

$$k_{j+1} = \frac{(1 + 2\sqrt{2}\, s_{j+1} + s_{j+1}^2)}{1 - s_{j+1}}\, k_j + \frac{2^j}{\sqrt{2}}\, \frac{s_{j+1}\left(1 - \frac{s_{j+1}}{\alpha}\right)(1 + 2\sqrt{2} + 2s_{j+1} - s_{j+1}^2)}{(1 - s_{j+1})(1 + \alpha s_{j+1})}.$$

Then k_j^{-1} converges quadratically to π.

Proof outline. By [2, p. 120, (1.2)] or [12, Theorem 2.1], we have

$$\frac{1}{u} - u = \frac{\varphi(q^2)}{q^{1/2}\psi(q^4)},$$

therefore by (2.4) and (2.3) we obtain

$$\frac{1}{u} - 2 - u = \frac{\varphi(q^2) - 2q^{1/2}\psi(q^4)}{q^{1/2}\psi(q^4)} = \frac{\varphi(-q^{1/2})}{q^{1/2}\psi(q^4)} = \frac{\eta^2(\tau/2)\eta(4\tau)}{\eta(\tau)\eta^2(8\tau)}. \tag{8.1}$$

This is an analogue of the results for u_n in Theorem 3.1. The procedure in Section 3 can now be followed, and we obtain

$$\frac{1}{w} - 6 + w = \frac{\eta^4(\tau)\eta^2(4\tau)}{\eta^2(2\tau)\eta^4(8\tau)},$$

$$u(e^{-\pi/2t}) = \frac{\alpha - u(e^{-2\pi t})}{1 + \alpha u(e^{-2\pi t})}, \qquad w(e^{-\pi/4t}) = \frac{\alpha^2 - w(e^{-2\pi t})}{1 - \alpha^2 w(e^{-2\pi t})};$$

$$(1 - \alpha^2 w(q_1))(1 - \alpha^2 w(q_2)) = 1 - \alpha^4$$

where

$$q_1 = \exp(-2\pi\sqrt{t}/\sqrt{N}), \qquad q_2 = \exp(-2\pi/\sqrt{Nt}), \qquad N = 8;$$

and

$$v = \frac{\alpha - \left(\frac{\alpha^2 - w}{1-\alpha^2 w}\right)^{1/2}}{1 + \alpha\left(\frac{\alpha^2 - w}{1-\alpha^2 w}\right)^{1/2}}, \qquad w = v\,\frac{1-v}{1+v}.$$

The last formula involving w and v was given in [12, Theorem 2.2].

Next, define $z = z(q)$, $A = A(q)$ and $M = M(q)$ by

$$z = 2q\,\frac{d}{dq}\log u_2, \qquad A = \frac{z}{1-u^2/\alpha^2}, \qquad M = \frac{A(q)}{A(q^2)}.$$

The analogue of Theorem 4.1 is

$$z = \frac{\eta^2(\tau)\eta(2\tau)\eta^3(4\tau)}{\eta(8\tau)^2} = \varphi(-q)\varphi(-q^2)\varphi^2(-q^4).$$

See [15, Theorem 3.1] for a proof and connections with sums of squares and sums of triangular numbers. The analogues of Theorems 4.3 and 4.4 are

$$M = \frac{1+2\sqrt{2}\,v+v^2}{1-v},$$

and

$$\frac{1}{MA(q^2)}\,q\,\frac{dM}{dq} = \frac{v}{M}\left(1-\frac{v^2}{\alpha^2}\right)\frac{dM}{dv}.$$

The analogues of Theorem 4.5 are

$$tA(e^{-2\pi\sqrt{t/N}}) = A(e^{-2\pi/\sqrt{Nt}})$$

and

$$\sqrt{t}\,\frac{\widetilde{A}}{A}\,(e^{-2\pi\sqrt{t/N}}) + \frac{1}{\sqrt{t}}\,\frac{\widetilde{A}}{A}\,(e^{-2\pi/\sqrt{Nt}}) = \frac{\sqrt{N}}{\pi},$$

with $N = 8$. Let

$$\kappa(t) = \frac{1}{\pi A} - 2\sqrt{\frac{t}{N}}\,\frac{\widetilde{A}}{A^2}$$

where

$$A = A(q), \qquad \widetilde{A} = q\,\frac{dA}{dq}, \qquad q = \exp(-2\pi\sqrt{t/N}), \qquad N = 8,$$

and define sequences $\{k_j\}$ and $\{s_j\}$ by

$$k_j = \kappa(2^{2j}) \quad \text{and} \quad s_j = u(e^{-2\pi\cdot 2^j/\sqrt{8}}) = u(e^{-2^j\pi/\sqrt{2}}).$$

Now follow the procedure at the end of Section 7 to show that these sequences have the properties claimed in Theorem 8.1. ∎

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Shaun Cooper
Institute of Information and Mathematical Sciences
Massey University
Private Bag 102904
North Shore Mail Centre
Auckland, New Zealand
E-mail: s.cooper@massey.ac.nz

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