Resolution of the Quinn–Rand–Strogatz Constant of Nonlinear Physics

D. H. Bailey, J. M. Borwein, and R. E. Crandall

CONTENTS

Herein we develop connections between zeta functions and some recent "mysterious" constants of nonlinear physics. In an important analysis of coupled Winfree oscillators, Quinn, Rand, and Strogatz [Quinn et al. 07] developed a certain N-oscillator scenario whose bifurcation phase offset small ϕ is implicitly defined, with a conjectured asymptotic behavior $\sin\phi \sim 1 - c_1/N$, with experimental estimate $c_1 = 0.605443657\ldots$. We are able to derive the exact theoretical value of this "QRS constant" c_1 as a real zero of a particular Hurwitz zeta function. This discovery enables, for example, the rapid resolution of c_1 to extreme precision. Results and conjectures are provided in regard to higher-order terms of the $\sin\phi$ asymptotic, and to yet more physics constants emerging from the original QRS work.

1. THE QRS CONSTANT

In a recent treatment, D. Quinn, R. Rand, and S. Strogatz, in describing a nonlinear Winfree-oscillator mean-field system, cite a formula

$$0 = \sum_{i=1}^{N} \left(2\sqrt{1 - s^2(1 - 2(i-1)/(N-1))^2} - \frac{1}{\sqrt{1 - s^2(1 - 2(i-1)/(N-1))^2}} \right), \qquad (1\text{–}1)$$

implicitly defining a phase offset angle $\phi := \sin^{-1} s$ due to bifurcation.[1] The authors conjectured, on the basis of numerical evidence, the asymptotic behavior of the N-dependent solution s to be

$$s \sim 1 - \frac{c_1}{N},$$

where c_1 is what we shall call the QRS constant, having—said those original authors—the empirical value $0.60544365\ldots$. Note the important fact that the very

[1] The QRS treatment [Quinn et al. 07] has $s = \sin\phi_0(1)$ in those authors' notation [Quinn et al. 07, p. 6].

2000 AMS Subject Classification: Primary 11Y60; Secondary 11M06

Keywords: Winfree oscillators, high-precision arithmetic, Hurwitz zeta, Richardson extrapolation

1058-6458/2009 $ 0.50 per page

existence of c_1 as a constant limit should be proven, and that is one of our present aims.

The present treatment began when we attempted to compute c_1 to significantly higher precision, so that the tools of experimental mathematics could be brought to bear on the problem [Bailey et al. 07, Borwein and Bailey 04, Borwein et al. 04]. Our experience shows that extreme-precision evaluation of constants that arise in mathematics or mathematical physics can be of enormous help, even if the constants are not discovered from the digits directly.[2] Extreme precision brings confidence during the sometimes arduous empirical verification of analytical results.

Our computational approach was as follows. Hoping to obtain a numeric value accurate to at least 40 decimal digits, we employed a software package that facilitates computations to 64-digit arithmetic (see the appendix, Section 6). We first rewrote the right-hand side of (1–1) by substituting $x = N(1 - s)$, so that the roots of the resulting function $F_N(x)$ directly correspond to approximations to c_1. Given a particular value of N, we found the root of $F_N(x)$ using iterative linear interpolation, in the spirit of Newton–Raphson iterations, until two successive values differed by no more than 10^{-52}. In this manner we found a sequence of roots x_m for $N = 4^m$, where m ranged from 1 to 15. These successive roots were then extrapolated to the limit as $m \to \infty$ (or in other words, as $N \to \infty$) using Richardson extrapolation [Sidi 02, pp. 21–41], in the following form:

For each $m \geq 1$, set $A_{m,1} = x_m$. Then for $k = 2$ to $k = m$, successively set

$$A_{m,k} = \frac{2^k A_{m,k-1} - A_{m-1,k-1}}{2^k - 1}. \tag{1–2}$$

This recursive scheme generates a triangular matrix A. The best estimates for the limit of x_m are the diagonal values $A_{m,m}$. Indeed, we found to our delight that for each successive m, the value $A_{m,m}$ agreed with $A_{m-1,m-1}$ to an additional three to four digits, which indicates that this extrapolation scheme is very effective on this problem.

In general, Richardson extrapolation employs a multiplier r, where we have used two in the numerator and denominator of (1–2), which multiplier r depends on the nature of the sequence being extrapolated. We found that two is the optimal value to use here quite by accident—what we actually discovered is that $\sqrt{2}$ is the optimal multiplier when $N = 2^m$, which implies that two is optimal when $N = 4^m$. The resulting final extrapolated value $A_{15,15}$ we obtained for $m = 15$ (corresponding to $N = 4^{15} = 1073741824$) is

$$c_1 \approx 0.6054436571967327494789228424472074752208996. \tag{1–3}$$

Since this and $A_{14,14}$ differed by only 10^{-38}, and successive values of $A_{m,m}$ had been agreeing to roughly four additional digits with each increase of m, we inferred that this numerical value was most likely good to 10^{-42}, or in other words, to the precision shown, except possibly for the final digit.

We then attempted to recognize this numeric value using the Inverse Symbolic Calculator tool.[3] Sadly, this tool was unable to determine any likely closed form.

After this recognition failure, we explored some analytic lemmas in the hope of giving the QRS constant a theoretical meaning. Indeed, in our case, the lack of immediate numerical discovery led to eventual theoretical success. We should also mention that having a suspected "moderate-precision" value such as the 42-digit entity above is of considerable aid during numerical testing of any theory. Moreover, another "mystery constant" we call C in our last section was found in closed form because of lucky manual experiments on such a moderate-precision value.

2. BOUNDING LEMMAS

We first simplify the nomenclature, noting that an equivalent formulation to the original work, now for $M := N - 1$ a positive integer, involves a sum

$$\mathcal{P}_N(s) := \sum_{k=0}^{M} \left(2\sqrt{1 - s^2(1 - 2k/M)^2} - \frac{1}{\sqrt{1 - s^2(1 - 2k/M)^2}} \right). \tag{2–1}$$

With this new nomenclature, consider a zero s_N having $\mathcal{P}_N(s_N) = 0$. We choose to state the QRS conjecture in the following form: Such a zero s_N exists, is unique on the positive reals, and enjoys a natural expansion

$$\frac{M}{s_N} - M \sim d_1 + \frac{d_2}{M} + \frac{d_3}{M^2} + \cdots$$

[2]By "extreme precision" is meant, in the spirit of previous papers such as [Bailey et al. 06], that "enough digits for detection" are obtained. In modern times, this means hundreds or thousands of digits, depending on the scope of search.

[3]Available online at http://oldweb.cecm.sfu.ca/projects/ISC/ISCmain.html. A new version of the ISC is available at http://ddrive.cs.dal.ca/~isc/.

with the coefficients d_j being absolute constants.[4] The establishment of this form leads immediately to a QRS expansion

$$1 - s_N \sim \frac{c_1}{N} + \frac{c_2}{N^2} + \frac{c_3}{N^3} + \cdots ,$$

with corresponding absolute constants c_j, therefore with

$$c_1 = d_1$$

the QRS constant, and higher coefficients derivable with series algebra. For example,

$$c_2 = d_1 - d_1^2 + d_2,$$
$$c_3 = d_1 - 2d_1^2 + d_1^3 - 2d_2 - 2d_1 d_2 + d_3,$$

and so on.

We shall be able to prove existence and uniqueness of s_N, and also prove that the QRS constant $d_1 = c_1$ exists as a genuine limit of $(M/s_N - M)$, with conjectures finally posited in regard to the higher-order d_j, c_j. The next lemmas serve to establish bounds crucial to such analysis.

Lemma 2.1. *Let $N > 1$ be a fixed integer, and consider real, positive arguments s. Then $\mathcal{P}_N(s)$ is strictly monotone decreasing in s, with $\mathcal{P}_N(0) = N$ and $\mathcal{P}_N(1) = -\infty$, so that for every $N > 1$ a unique zero s_N always exists; in fact, $s_N \in (0, 1)$.*

Proof: The monotonicity is obvious from the radicals in the summand; in fact, each summand is itself strictly monotonic decreasing in s, except for a possible harmless constant summand when M is even and $k = M/2$. Also immediate are the endpoint values of $\mathcal{P}_N$ for $s = 0, 1$. □

To further facilitate asymptotic analysis, we shall establish a reasonably tight bound on the unique zero s_N of Lemma 2.1. We shall use an elementary form of the Euler–Maclaurin summation formula valid for any continuously differentiable function f on the real interval (a, b) [Atkinson 93, p. 285], [Titchmarsh 51, (2.1.2)]; namely, denoting by $W(x) := x - \lfloor x \rfloor - \frac{1}{2}$ the antisymmetric sawtooth function, we have

$$\sum_{a<k\le b} f(k) = \int_a^b f(x)\,dx + \int_a^b W(x) f'(x)\,dx + W(a)f(a) - W(b)f(b). \qquad (2\text{–}2)$$

[4]We admit that our use of the term "natural" is based on hindsight; the given expansion with the d_j occurs naturally in our subsequent analysis.

The bounding scheme we have in mind runs as follows:

Lemma 2.2. *For positive integer $M := N - 1$, the real positive zero s_N satisfies*

$$1 > s_N > 1 - \frac{28}{27}\frac{1}{M},$$

as well as

$$0 < \frac{M}{s_N} - M < \frac{20}{19}.$$

Remark 2.3. These effective bounds are true, regardless of any expansion for s_N. The lemma does, however, prove that if the QRS constant c_1 exists, then said constant must be in $\left(0, \frac{28}{27}\right)$.

Proof: Define $T := \lfloor M/2 \rfloor$ and write

$$\mathcal{P}_N(s) = -\delta_{M,\text{ even}} + 2\sum_{k=0}^{T}\left(2\sqrt{1 - s^2(1-2k/M)^2} - \frac{1}{\sqrt{1 - s^2(1-2k/M)^2}}\right). \qquad (2\text{–}3)$$

We now identify $a := 0, b := M/2$, and

$$f(x) := 2\sqrt{1 - s^2(1-2x/M)^2} - \frac{1}{\sqrt{1 - s^2(1-2x/M)^2}}$$

in the identity (2–2), where all right-hand terms are easy except for the second integral, which we bound on the knowledge that this f is monotone increasing over $x \in [0, M/2]$:

$$\left| \int_0^{M/2} W(x) f'(x)\,dx \right| \le \frac{1}{2}(f(M/2) - f(0)).$$

These machinations yield, whether M be even or odd,

$$\mathcal{P}_N(s) > -1 + 4\sqrt{1-s^2} - \frac{2}{\sqrt{1-s^2}} + M\sqrt{1-s^2}. \qquad (2\text{–}4)$$

A zero of the right-hand side of (2–4) is

$$s' = \sqrt{1 - \left(\frac{1 + \sqrt{8M+33}}{2M+8}\right)^2}.$$

It is straightforward to check the derivative ds'/dM and the value of s' at the critical point to conclude that $s' > 1 - \frac{28}{27}/M$, so the first result of the lemma follows. The second result follows from similar critical-point analysis of $M/s' - M$. □

3. POISSON TRANSFORMATION

It is tempting, on the basis of Lemma 2.2, to explore tighter theoretical bounds, say via Euler–Maclaurin formulas or the like. Unfortunately, such an approach has various problems stemming from the manifestly asymptotic nature of Euler–Maclaurin error terms. Instead, we have opted for a Poisson transformation of the $\mathcal{P}$ sum.

For a wide class of functions f one has the Poisson identity

$$\sum_{k\in Z} f(k) = \sum_{n\in Z} \int_{-\infty}^{\infty} f(x) e^{2\pi i n x}\, dx. \tag{3–1}$$

This holds for any Lebesgue integrable function [Borwein and Bailey 04, Theorem 2.12]. Generally speaking, if the left-hand sum is, as in our case for $\mathcal{Q}$, to be truncated at finite limits, then we may use the relation

$$\sum_{k=0}^{M} f(k) = \sum_{n\in Z} \int_{-\eta}^{M+\eta} f(x) e^{2\pi i n x}\, dx, \tag{3–2}$$

provided that $\eta \in (0, 1)$. This "truncated" Poisson expansion can be proved directly, for example via standard techniques such as summation formulas. One may establish the Poisson transformation, for example, using (2–2) and integrating by parts, employing at a key step a Fourier series for the sawtooth function W [Titchmarsh 51, (2.1.7)]. Any integrable ($f \in L_1$) function with finite-interval support allows the transformation, or by applying (3–1) to f restricted to $[-\eta, M + \eta]$.

Theorem 3.1. *Let $M := N - 1$ be a positive integer, and assume for a positive real s that $0 < M/s - M < 2$. Then we have the identity*

$$\mathcal{P}_N(s) = \frac{\pi M}{s} \sum_{n=1}^{\infty} (-1)^{nM} J_2\left(\frac{\pi n M}{s}\right), \tag{3–3}$$

where J_2 is the standard Bessel function of order 2.

Proof: For the real s assumed, we can, according to Lemma 2.2, take $\epsilon := M/s - M \in (0, 2)$ and infer

$$\mathcal{P}_N(s) = \sum_{n\in Z} \int_{-\epsilon/2}^{M+\epsilon/2} e^{2\pi i n x} \left(2\sqrt{1 - s^2(1 - 2x/M)^2} - \frac{1}{\sqrt{1 - s^2(1 - 2x/M)^2}}\right) dx.$$

Setting $x \mapsto (M/2)(1 - (1/s)\cos t)$, we have

$$\begin{aligned}\mathcal{P}_N(s) &= \sum_{n\in Z} \frac{M}{s} e^{i\pi n M} \int_0^{\pi} dt\, \left(1 - 2\sin^2 t\right) e^{-\pi i n \frac{M}{s}\cos t} \\ &= \frac{M}{s} \sum_{n\in Z} e^{i\pi n M} \int_0^{\pi} \cos(2t)\, e^{-\pi i n \frac{M}{s}\cos t}\, dt \\ &= \frac{\pi M}{s} \sum_{n=1}^{\infty} (-1)^{nM} J_2\left(\frac{\pi n M}{s}\right),\end{aligned} \tag{3–4}$$

where the final equation (3–4) follows from the representation for J_2 in [Ambramowitz and Stegun 65, equation 9.2.21], since J_2 is an even function with $J_2(0) = 0$. □

4. ASYMPTOTIC ANALYSIS

Evidently, our sought-after zero s_N for the QRS problem solves

$$0 = \sum_{n=1}^{\infty} J_2\left(\frac{\pi n M}{s_N}\right) (-1)^{nM}, \tag{4–1}$$

and has a proven constraint; namely, if we write

$$\frac{M}{s_N} = M + \delta_N,$$

then $0 < \delta_N < \frac{20}{19}$. Simple as the Bessel-sum relation may appear, it contains clues as to the difficulty of our desired asymptotic analysis. Indeed, the Bessel function exhibits damped oscillation, and the arithmetic progression $\{\pi n M/s_N : n = 1, 2, 3, \ldots\}$ samples said oscillations in somewhat chaotic fashion, at least until the Bessel argument is large.

To address the issue of oscillations in such summands, we state a classical truth in regard to the Bessel function: For positive real z,

$$\begin{aligned}J_2(z) = \sqrt{\frac{2}{\pi z}} &\left(\cos(z - 5\pi/4) - \frac{15}{8z}\sin(z - 5\pi/4)\right) \\ &+ O\left(z^{-5/2}\right).\end{aligned} \tag{4–2}$$

This kind of asymptotic is presented in most references that explain Bessel functions, say [Ambramowitz and Stegun 65, p. 364]. However, if one desires effective bounds, that is, explicit big-O constants, the reference [Borwein et al. 07] provides a method for effective bounds (and convergent—not asymptotic—series) for $J_n(z)$, with n any integer.

Compelled by the appearance of the cos–sin terms in the Bessel asymptotic (4–2), we define a set of *offset-periodic zeta functions*:

$$\begin{aligned}\mathcal{Q}_s(z) &:= \sum_{n=1}^{\infty} \frac{\cos(\pi n z - 5\pi/4)}{n^s} \\ &= -\frac{1}{\sqrt{2}} \left\{ \sum_{n=1}^{\infty} \frac{\cos(\pi n z)}{n^s} + \sum_{n=1}^{\infty} \frac{\sin(\pi n z)}{n^s} \right\}, \\ \mathcal{R}_s(z) &:= \sum_{n=1}^{\infty} \frac{\sin(\pi n z - 5\pi/4)}{n^s} \\ &= \frac{1}{\sqrt{2}} \left\{ \sum_{n=1}^{\infty} \frac{\cos(\pi n z)}{n^s} - \sum_{n=1}^{\infty} \frac{\sin(\pi n z)}{n^s} \right\}.\end{aligned}$$

For positive real s and for z not an even integer, these summations are all seen—by a standard uniform Abel test—to converge to continuous functions. The functions also enjoy polylogarithmic forms, at least for real s:

$$\mathcal{Q}_s(z) = -\frac{1}{\sqrt{2}} \left(\operatorname{Re} \operatorname{Li}_s\left(e^{i\pi z}\right) + \operatorname{Im} \operatorname{Li}_s\left(e^{i\pi z}\right) \right), \tag{4–3}$$

$$\mathcal{R}_s(z) = \frac{1}{\sqrt{2}} \left(\operatorname{Re} \operatorname{Li}_s\left(e^{i\pi z}\right) - \operatorname{Im} \operatorname{Li}_s\left(e^{i\pi z}\right) \right). \tag{4–4}$$

Here $\operatorname{Li}_s(z) := \sum_{n=0}^{\infty} z^n/n^s$ for $|z| < 1$ and its analytic continuation for other z [Lewin 81]. For example, $Q_s(z) = 0$ can be solved with polylogarithm calculations, using the first of these two relations. Of special interest now is the Erdélyi expansion [Erdéyli 53, vol. 1, p. 29], [Crandall and Buhler 95]:

$$\operatorname{Li}_s\left(e^{i\pi z}\right) = \Gamma(1-s)(-i\pi z)^{s-1} + \sum_{m \geq 0} \frac{\zeta(s-m)}{m!}(i\pi z)^m, \tag{4–5}$$

valid on $z \in (0, 2)$, with s not a positive integer (in which case, canceling divergences can be analyzed to recast the right-hand side). We may employ the Riemann functional equation, which stipulates that

$$\pi^{-s/2}\Gamma(s/2)\zeta(s)$$

is invariant under $s \mapsto 1 - s$, to convert all ζ arguments into positive ones. Putting all of this together for the case $s = \frac{1}{2}$, we obtain

$$\mathcal{Q}_{1/2}(z) = -\frac{1}{\sqrt{z}} + \sum_{n \geq 0} q_n z^n, \tag{4–6}$$

where the coefficients enjoy a closed form

$$q_m := -\frac{1}{\sqrt{2}}\zeta\left(m + \frac{1}{2}\right) \prod_{k=1}^{m} \left(\frac{1}{4k} - \frac{1}{2}\right).$$

(An empty product is interpreted as 1.) It is fascinating that starting with q_1, the coefficients in (4–6) are alternating in sign. Indeed, an alternative series for $\mathcal{Q}_{1/2}$ is given by

$$\mathcal{Q}_{1/2}(z) = -\frac{1}{\sqrt{z}} - \frac{1}{\sqrt{2}} \sum_{n=0}^{\infty} \zeta\left(n + \frac{1}{2}\right) \binom{2n}{n} \left(-\frac{z}{8}\right)^n. \tag{4–7}$$

There is another vantage point on the $\mathcal{Q}, \mathcal{R}$ pair. Namely, since the polylogarithmic Li_s is a case of the Lerch zeta function, and since there is a functional equation for the Lerch, one may work out, from (4–3), (4–4), and a suitable reference [Laurincikas and Garunkstis 02, Section 2.2] a functional relation

$$\begin{aligned}&\operatorname{Li}_s\left(e^{i\pi z}\right) \\ &\quad = i(2\pi)^{s-1}\Gamma(1-s) \qquad\qquad (4\text{–}8)\\ &\qquad \times \left\{ e^{-i\pi s/2}\zeta\left(1-s, \frac{z}{2}\right) - e^{i\pi s/2}\zeta\left(1-s, 1-\frac{z}{2}\right) \right\},\end{aligned}$$

where now $\zeta(s, a) := \sum_{n \geq 0} 1/(n+a)^s$ is the Hurwitz zeta function. Formula (4–8) is valid for all $z \in (0, 2)$ and for any complex s for which the right-hand side exists as an analytic continuation. In turn, $\zeta(s, a)$ can be analytically continued except for a pole at $s = 1$, so (4–8) has a wide scope of validity. For our present purposes, the functional equation proves, for real s, via (4–3), (4–4), the following lemma.

Lemma 4.1. *For real s, z with $z \in (0, 2)$ we have the following functional relations for the offset-periodic zeta functions $\mathcal{Q}, \mathcal{R}$ and the Hurwitz zeta function, all entities being analytic continuations:*

$$\begin{aligned}\mathcal{Q}_s(z) &= -(2\pi)^{s-1}\Gamma(1-s) \\ &\quad \times \left\{ \zeta\left(1-s, \frac{z}{2}\right) \cos\left(\frac{(2s-1)\pi}{4}\right) \right. \\ &\qquad \left. + \zeta\left(1-s, 1-\frac{z}{2}\right) \sin\left(\frac{(2s-1)\pi}{4}\right) \right\}, \\ \mathcal{R}_s(z) &= (2\pi)^{s-1}\Gamma(1-s) \\ &\quad \times \left\{ \zeta\left(1-s, 1-\frac{z}{2}\right) \cos\left(\frac{(2s-1)\pi}{4}\right) \right. \\ &\qquad \left. + \zeta\left(1-s, \frac{z}{2}\right) \sin\left(\frac{(2s-1)\pi}{4}\right) \right\}.\end{aligned}$$

Note that for half-odd s such as $s = -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$, there is precisely one Hurwitz zeta function in play. Special instances of Lemma 4.1 are thus

$$\mathcal{Q}_{-1/2}(z) = \frac{1}{\pi\sqrt{32}}\,\zeta\left(\frac{3}{2}, 1-\frac{z}{2}\right),$$

$$\mathcal{Q}_{1/2}(z) = -\frac{1}{\sqrt{2}}\,\zeta\left(\frac{1}{2}, \frac{z}{2}\right),$$

$$\mathcal{Q}_{3/2}(z) = \pi\sqrt{8}\,\zeta\left(-\frac{1}{2}, 1-\frac{z}{2}\right),$$

$$\mathcal{R}_{-1/2}(z) = -\frac{1}{\pi\sqrt{32}}\,\zeta\left(\frac{3}{2}, \frac{z}{2}\right),$$

$$\mathcal{R}_{1/2}(z) = \frac{1}{\sqrt{2}}\,\zeta\left(\frac{1}{2}, 1-\frac{z}{2}\right),$$

$$\mathcal{R}_{3/2}(z) = -\pi\sqrt{8}\,\zeta\left(-\frac{1}{2}, \frac{z}{2}\right).$$

There is one more foray we require before proving the main asymptotic conjecture. We shall employ the following representation for the analytic continuation of the Hurwitz zeta function:

Lemma 4.2. [Crandall 08] *The complete analytic continuation of $\zeta(s,a)$ for $a \in (0,1)$, $s \neq 1 + 0i$, is given by*

$$\zeta(s,a) = \frac{1}{\Gamma(s)}\sum_{n\geq 0}\frac{\Gamma(s,\lambda(n+a))}{(n+a)^s} + \frac{1}{\Gamma(s)}\sum_{m\geq 0}\frac{(-1)^m B_m(a)}{m!}\,\frac{\lambda^{m+s-1}}{m+s-1},$$

with the following interpretations: $\Gamma(s,\cdot)$ is the standard incomplete gamma function, B_n is the standard Bernoulli polynomial, λ is a free parameter with $|\lambda| < 2\pi$. For any case of integer $s = -n \leq 0$, the $\Gamma(s)$ divergence cancels a divergent m-summand, and so $\zeta(-n,a) = -B_{n+1}(a)/(n+1)$.

Though Lemma 4.2 was developed for computational purposes, there is one useful side result:

Corollary 4.3. *If $s \neq 1$ is positive real, the formal derivative relation*

$$\frac{\partial}{\partial a}\zeta(s,a) = -s\zeta(s+1,a)$$

holds, even if the left-hand side is the analytic continuation (the right-hand side being always a convergent sum).

Proof: From the relation of Lemma 4.2, with say $\lambda := 1$, both absolutely convergent sums can be differentiated internally. One may use $B'_m(x) = B_{m-1}(x)$ and the standard recurrence relation for $\Gamma(s,.)$. One sees that—remarkably enough—each sum has the derivative property specified for $\zeta(s,a)$ itself. □

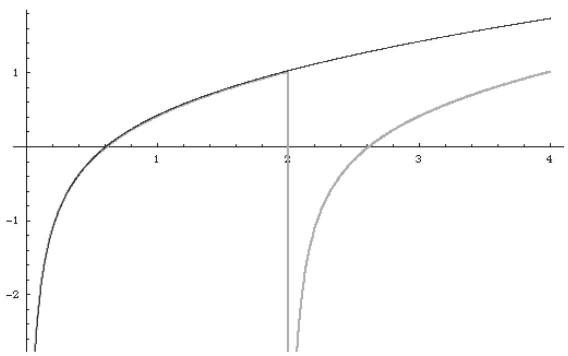

FIGURE 1. Plots of the offset-periodic and Hurwitz zeta functions $\mathcal{Q}_{1/2}(z)$ and $-\zeta\left(\frac{1}{2}, \frac{z}{2}\right)/\sqrt{2}$, respectively (vertical) vs. z (horizontal) on $(0,4)$. The $\mathcal{Q}_{1/2}$ function has a discontinuity at $z = 2$, to the left of which the two functions precisely coincide, are strictly monotone, and exhibit a zero $z_0 \approx 0.6$.

We are now prepared to establish certain key properties of the $\mathcal{Q}_{1/2}$ function (the reader may wish to refer to the graph in Figure 1):

Lemma 4.4. *For z belonging to the open interval $(0,2)$,*

(1) *$\mathcal{Q}_{1/2}(z)$ is infinitely differentiable,*

(2) *$\mathcal{Q}_{1/2}(z)$ is strictly monotone increasing,*

(3) *$\mathcal{Q}_{1/2}(z)$ has a unique zero, say z_0, i.e., $\mathcal{Q}_{1/2}(z_0) = 0$, which belongs in the subinterval $(0,1)$.*

Proof: From the closed form for the q_m coefficients, one can see that $|q_m| < 1/2^m$ for all $m \geq 0$. Thus for any $|z| < 2$, the given series converges, as does the series for any order of derivative of $\mathcal{Q}_{1/2}$, thus settling part (1). (One could also use the corollary to Lemma 4.2 to infer arbitrary differentiability.)

For part (2), observe that Corollary 4.3 assures us that the derivative of $\mathcal{Q}_{1/2}(z) = -\zeta\left(\frac{1}{2}, \frac{z}{2}\right)/\sqrt{2}$ is positively proportional to $\zeta\left(\frac{3}{2}, \frac{z}{2}\right)$, which itself is a manifestly positive convergent sum. Thus $\mathcal{Q}_{1/2}$ has positive slope over the interval.

For part (3), it is an easy check that for $z \to 0^+$, the function $\mathcal{Q}_{1/2}$ diverges negatively as $-z^{-1/2}$. On the other hand, it is an easy (and effectively boundable) check that $\mathcal{Q}_{1/2}(1) > 0$. For example,

$$\mathcal{Q}_{1/2}(1) > -1 - \frac{\zeta\left(\frac{1}{2}\right)}{\sqrt{2}} + \frac{5\zeta\left(\frac{3}{2}\right)}{32\sqrt{2}} > 0.3.$$

(See text below for the closed form for $\mathcal{Q}_{1/2}(1)$.) Therefore a zero-crossing exists and is unique by part (2). □

We are finally in a position to resolve the QRS constant, as follows:

Theorem 4.5. *The sequence* $\{\delta_N := M/s_N - M : M \in Z^+\}$ *approaches a definite limit, said limit being the zero* z_0 *of Lemma 4.4, and so the QRS constant* c_1 *exists and is the unique zero of the Hurwitz zeta function* $\zeta\left(\frac{1}{2}, \frac{z}{2}\right)$ *on* $z \in (0, 2)$.

Proof: Write the Bessel asymptotic (4–2) as

$$J_2(z) = \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{5\pi}{4}\right) + O\left(z^{-3/2}\right),$$

and then observe that

$$\begin{aligned}
&\sum_{n\geq 1} J_2(\pi n M/s_N) e^{i\pi n M} \\
&\quad = \frac{1}{\pi}\sqrt{\frac{2s_N}{M}} \sum_{n\geq 1} \frac{(-1)^{nM}}{\sqrt{n}} \cos\left(\pi n (M + \delta_N) - \frac{5\pi}{4}\right) \\
&\qquad + O\left(\frac{1}{M^{3/2}} \sum_{n\geq 1} \frac{1}{n^{3/2}}\right) \\
&\quad = \frac{1}{\pi}\sqrt{\frac{2s_N}{M}} \sum_{n\geq 1} \frac{1}{\sqrt{n}} \cos\left(\pi n \delta_N - \frac{5\pi}{4}\right) + O\left(\frac{1}{M^{3/2}}\right).
\end{aligned}$$

But the Bessel sum vanishes for every δ_N, so we must have

$$\mathcal{Q}_{1/2}(\delta_N) = O\left(\frac{1}{M}\right).$$

Now the point of our previous analytical results on $\mathcal{Q}_{1/2}$ for the open interval $(0, 2)$ is apparent: We know from Lemmas 2.2 and 4.4 that $\mathcal{Q}_{1/2}$ has a legitimate inverse over the entire domain $\left(-\infty, -\zeta\left(\frac{1}{2}\right)/\sqrt{2}\right]$, which domain contains the full sequence $\{\delta_N\}$. We can write

$$\delta_N = {\mathcal{Q}_{1/2}}^{-1}\left(O\left(\frac{1}{M}\right)\right),$$

so that our limit in fact exists, namely, $\lim \delta_N = z_0 = d_1 = c_1$. □

Using formula (4–3) for $\mathcal{Q}_{1/2}$, employing also a root-finding algorithm, we produced the 1500-digit value of the zero that appears in our appendix. We note that $\mathcal{Q}_{1/2}(2^-) = -\zeta\left(\frac{1}{2}\right)/\sqrt{2} = 1.0326265761156085\ldots$, as can be calculated by methods relevant to Lemma 4.1 but was also found using the Inverse Symbolic Calculator. Likewise,

$$\begin{aligned}
\mathcal{Q}_{1/2}(1) &= -\zeta\left(\frac{1}{2}\right)\left(1 - \frac{1}{\sqrt{2}}\right) \\
&= 0.42772793269397822\ldots.
\end{aligned}$$

5. HIGHER-ORDER ASYMPTOTICS

On the matter of the coefficient d_2, which immediately yields a c_2, again we took the experimental-mathematical path. First, we established via similar extrapolation to that for c_1 the estimate

$$c_2 \approx -0.104685459433071176262158436589.$$

Then, by analyzing the Bessel asymptotic (4–2) through the sine term inclusive, we found (and hereby omit the tedious derivation) that

$$d_2 = -\frac{15}{16\pi^2}\frac{\mathcal{R}_{3/2}(z_0)}{\mathcal{R}_{-1/2}(z_0)},$$

and thus, with z_0 again being the zero of $\zeta\left(\frac{1}{2}, \frac{z}{2}\right)$, we established a closed form for c_2:

$$c_2 = z_0 - z_0^2 - 30\frac{\zeta\left(-\frac{1}{2}, \frac{z_0}{2}\right)}{\zeta\left(\frac{3}{2}, \frac{z_0}{2}\right)}. \qquad (5\text{–}1)$$

It is a delight that this value for c_2—found in our appendix to extreme precision—agrees with the above extrapolation value. But perhaps most interesting is this: Whereas c_1 was an "implicit solution," i.e., a Hurwitz-zeta zero, it turns out that c_2 is just an "evaluation" involving said zero. We do not yet know whether higher-order c_j will take the form of implicit zeros, or evaluations. For such higher-order analysis, the complications arise in the fact that the formal series for $M/s_N - M$ appears in both the asymptotic powers and the cos/sin terms of the general Hankel asymptotic for J_2. It may help to use absolutely convergent series for J_2, as found in [Borwein et al. 07]. These special series, sometimes called Hadamard series (see the given reference for distinctions), are not the classical ascending series, which do converge; they are series structured just like the asymptotic series but that nevertheless converge absolutely.

We would like to conjecture that the d_j coefficients are bounded, and so are the c_j. This happy circumstance would mean, of course, that the so-called asymptotic series is really a convergent series, and such a phenomenon is at least consistent with the bounding lemma Lemma 2.2.

Finally, we also identified another constant conjectured in the Quinn–Rand–Strogatz paper [Quinn et al. 07, equation 55]. Therein the authors define a function S by

$$S(N,a) := \sum_{i=1}^{N} \left[1 - a^2\left(1 - \frac{2i-2}{N-1}\right)^2\right]^{-3/2}$$

and then note that the limit

$$C = \lim_{N\to\infty} \frac{S(N, 1-c_1/N)}{N^{3/2}} = 2.038169\ldots$$

appears to hold, although they admit having neither an exact value nor a proof of existence for the constant.

To resolve these matters, we first obtained 43-digit accuracy, by means, again, of a high-precision Richardson extrapolation scheme. Our result is

$$C \approx 2.038169379702150621710648459728295516278714 0.$$

Guided by this experimental number, we were able to guess (literally, by hand) an exact form by noticing that the 43-digit C value satisfies, to the implied accuracy,

$$\frac{C}{\zeta\left(\frac{3}{2}, \frac{c_1}{2}\right)} = 0.250000000000000000000000000000000000000000\ldots,$$

where c_1 is what we have been calling all along the QRS constant.

Rather than developing here a full theorem in regard to existence (of C) and closed-form value

$$C = \frac{1}{4}\zeta\left(\frac{3}{2}, \frac{c_1}{2}\right) = -\frac{\partial}{\partial a}\zeta\left(\frac{1}{2}, \frac{a}{2}\right)\Big|_{a=c_1}, \tag{5–2}$$

we shall, for the sake of brevity, merely sketch the argument. First, rewrite the S definition as

$$S(N,a) = -\delta_{M \text{ even}} + 2\sum_{k=0}^{\lfloor M/2\rfloor}\left[1 - a^2\left(1 - \frac{2k}{M}\right)^2\right]^{-3/2}, \tag{5–3}$$

where $M = N - 1$ as before. Now, roughly speaking (for this sketch we use "∼" rather loosely, heuristically, for large M) we have

$$a^2 \sim 1 - 2\frac{c_1}{M},$$

and for small k/M,

$$1 - a^2\left(1 - \frac{2k}{M}\right)^2 \sim \frac{2c_1 + 4k}{M},$$

so that we can rewrite (5–3) as

$$S \sim \frac{2M^{3/2}}{4^{3/2}} \sum_{k\geq 0} \frac{1}{(k + c_1/2)^{3/2}} = \frac{1}{4}\zeta\left(\frac{3}{2}, \frac{c_1}{2}\right) M^{3/2},$$

thus establishing (5–2).

It should be possible—if tedious—to work out in the above fashion arbitrary orders of the large-N expansion of $S(N, 1-c_1/N) \sim CN^{3/2} + O(N^2)$.

An extreme-precision value for C is exhibited in our appendix. Incidentally, we also believe that a theory of sums similar to S, but having, say, a denominator power s instead of $\frac{3}{2}$, with $\mathrm{Re}(s) > 1$, should be possible and surely would involve Hurwitz-zeta evaluations $\zeta(s,\cdot)$.

6. APPENDIX

The 42-digit extrapolation value (1–3) for c_1 was calculated using the "quad-double" (QD) package, which is described in the paper [Hida et al. 01] and is available at http://crd.lbl.gov/~dhbailey/mpdist. This software permits one to write conventional Fortran-90 or C++ programs, defining some or all variables to be of type `dd_real` (double-double precision, or roughly 32 decimal digits) or `qd_real` (quad-double precision, or roughly 63 decimal digits). Our code used the `qd_real` data type. While we developed this code on systems at the Lawrence Berkeley Laboratory, the final computations that produced this value, as well as those for c_2 and C, were performed on the Terascale Computing Facility, an Apple-based parallel computer at Virginia Tech (whom we thank for their generous grant of computer time). Each of these three runs used 64 CPUs and required a run of 25 minutes.

Once we found formula (4–3), we used the `FindRoot[ ]` function in Mathematica to obtain a 1500-decimal-digit value for the QRS constant c_1, shown in Table1:

We performed a similar extreme computation in Maple. This value agrees with the value we originally determined using Richardson extrapolation in equation (1–3), up through the penultimate digit of the latter.

0.605443657196732749478922842447207475220899496956322617877552877451828998351676356757047292138342704152364233857109663916913 90
262465433071327650822523319390084685432498169662517432691699389935790212911516277951448012658096317353530645845952560506335 6503
881353198442708331101924346932770089068731693179963014632131860092167473830897410170079865670753589502857108856618235333540 5921
652886974844346002926670517781741686176818017483543352378797702880483574067491652117216737990532059789423395594416138766678 7916
716482242423360949979690742320608766453918197220499525233843394521960566489388929801188508797430520369831410510154322153857 5519
816012495252663447410757151998316799848670504735254558239233528938993871822061596825693253743025390693658039474077646100883 5378
927133384884131428133608522737823790911326342919760897512801398336380219021008425837665411311346859291065380542948931698005 6244
999683185858405437877435116502065605780548341791983066067335370436898668853573865831986438379498480625999332856109443152412 7891
732082169017004287298759390807110643590128577439050915897934959875975994219962188580193113865548438958534740129282717872355 2313
686416679400496732724398645281318049205395359975228111566927152868448071109074725231099364462870585759813556902978872565904 1441
316785209327146704859154579529036325390447532826758763889071556055779428021858076930820373520294641066117662953901816524546 6244
7301630713439212117681586103054903158367238849822578085297095188604662478455941 4954886

TABLE 1. A 1500-decimal-digit value for the QRS constant c_1.

− 0.104685459433071176262158436583950361566306188422928659240897990324451611646049956678924019508712254741131782837113318385807 64
503659384455260680747280480919364062912336723121576669247369684086851908155279149809902932153332042942337222251994392457714 277470
417895645311497586529672299884948664410703210607989056878250005783690981299967383163468963529819148190754502985179083520734 517381
968612330700022244842141949379853225445020671384046971570119519442021100918009527214462372642876714506074324178996823633869 0043646
356239576319389604890876316488659231949305701716411742822220451754191278466550877434545428589049468919278630852476250406722 6003147
454666014520115403333406537828546515964142640936720948518815173556382284873978324896242696885926836453936874601493843020864 8300095
325906426554881222067194849966134503688713614554426855675253059310740053790054440559676485907250923561191206037643100270798 5999037
345580831405988651775997745988004892699896596361719001377875900107219982999835250170177194227551679304535912806909557679144 8908784
127177575137443744857126275856378606195130575290625807083268797803776195706822059911091567484752687574296416395795414617268 3855621
356903931078911099252702539362801402460202480060456473486104118239431522867943189668043263942778970951537359691407979040844 76

TABLE 2. An extreme-precision value for the second asymptotic coefficient c_2.

2.038169379702150621710648459728295516278713961805208070047044564382879711524651476868574278314962588666944434112853514044764 379850
340978257807316777555015041643976272359262917234698826027822459888955908521472888473377054757730819579450493523847922305208 03926215
380580285550602928396439829477893927167838150301642358124472845674632009705601454275376963643030927475660933529544899213036 60334802
844081413538201842814864727350456392328724904908909642037158255780316539311700396083119879377268429156711448843430471273241 91067113
149112569515436531583926816726289846634402116932782426646964816738813201418526878677025111971602051597783574841721311342362 315825613
059537931083602257420118953457179137130470099003408569476546732912452084291139014843029198934172701094463167864365403414806 83665456
861781522955319022948489493525358075042761950648761778251632537541659777136590014640121450007486011446029189620949274312909 60912626
46405482045837854677579756321017522873147050151942200456879486850004126873254128 2751

TABLE 3. An extreme-precision value for the ancillary constant C.

In a similar manner, we were able to compute an extreme-precision value for the second asymptotic coefficient c_2, using (5–1) and the above value for c_1 (which equals z_0). Our result is given in Table 2.

An extreme-precision value for the ancillary constant C, shown in Table 3, is a straightforward Hurwitz-zeta computation.

ACKNOWLEDGMENTS

The authors are very grateful to Steven Strogatz of Cornell University, who introduced us to this problem and gave us many encouraging words of support for the research. The first author was supported in part by the director, Office of Computational and Technology Research, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy, under contract number DE-AC02-05CH11231. The second author was supported in part by NSERC and the Canada Research Chair Programme.

REFERENCES

[Ambramowitz and Stegun 65] M. Ambramowitz and I. Stegun. *Handbook of Mathematical Functions*. New York: Dover, 1965.

[Atkinson 93] Kendall E. Atkinson. *Elementary Numerical Analysis*. New York: John Wiley and Sons, 1993.

[Bailey et al. 06] D. Bailey, J. Borwein, and R. Crandall, "Integrals of the Ising class." *J. Phys. A.: Math. Gen.* 39 (2006), 12271–12302.

[Bailey et al. 07] David H. Bailey, Jonathan M. Borwein, Neil J. Calkin, Roland Girgensohn, D. Russell Luke, and Victor Moll. *Experimental Mathematics in Action*. Wellesley: A K Peters, 2007.

[Borwein and Bailey 04] Jonathan Borwein and David Bailey. *Mathematics by Experiment: Plausible Reasoning in the 21st Century*. Wellesley: A K Peters, 2004.

[Borwein et al. 04] Jonathan Borwein, David Bailey, and Roland Girgensohn. *Experimentation in Mathematics: Computational Paths to Discovery*. Wellesley: A K Peters, 2004.

[Borwein et al. 07] D. Borwein, J. Borwein, and R. Crandall. "Effective Laguerre Asymptotics." *SIAM J. Numer. Anal.* 6 (2007), 3285-3312.

[Crandall 08] R. Crandall., "Unified Algorithms for Polylogarithm, L-Series, and Zeta Variants." Preprint, 2008.

[Crandall and Buhler 95] R. E. Crandall and J. P. Buhler. "On the Evaluation of Euler Sums." *Experimental Mathematics* 3:4 (1995) 275–285.

[Erdéyli 53] A. Erdéyli. *Higher Transcendental Functions*. New York: Mcgraw-Hill, 1953.

[Hida et al. 01] Yozo Hida, Xiaoye S. Li, and David H. Bailey. "Algorithms for Quad-Double Precision Floating Point Arithmetic." In *15th IEEE Symposium on Computer Arithmetic*, pp. 155–162. Los Alamitos: IEEE Computer Society, 2001.

[Laurincikas and Garunkstis 02] A. Laurincikas and R. Garunkstis. *The Lerch Zeta-Function*. Dordrecht: Kluwer, 2002.

[Lewin 81] L. Lewin. *Polylogarithms and Associated Functions*. Amsterdam: Elsevier North Holland, 1981.

[Quinn et al. 07] D. Quinn, R. Rand, and S. Strogatz. "Singular Unlocking Transition in the Winfree Model of Coupled Oscillators." *Phys. Rev E* 75 (2007), 036218-1-10.

[Sidi 02] Avram Sidi. *Practical Extrapolation Methods: Theory and Applications*. Cambridge: Cambridge University Press, 2002.

[Titchmarsh 51] E. Titchmarsh. *The Theory of the Riemann Zeta Function*. Oxford: Clarendon Press, 1951 (reprinted 1967).

D. H. Bailey, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 (dhbailey@lbl.gov)

J. M. Borwein, School of Mathematical & Physical Sciences, University of Newcastle Callaghan, NSW 2308, Australia (Jonathan.Borwein@newcastle.edu.au)

R. E. Crandall, Center for Advanced Computation, Reed College, Portland OR (crandall@reed.edu)

Received June 2, 2007; accepted January 18, 2008.