Resolution of the Quinn-Rand-Strogatz constant of nonlinear physics

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Abstract: 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 [14] developed a certain N-oscillator scenario whose bifurcation phase offset ϕ is implicitly defined, with a conjectured asymptotic behavior: $\sin \phi \sim 1 - c_1/N$, with experimental estimate $c_1 = 0.605443657...$ 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.

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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

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

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... Note the important fact that the very 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 [4][6][7]. Our experience shows that extreme-precision² 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. Moreover, 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 Appendix). We first rewrote the right-hand side of (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 $F_N(x)$ by 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 one to 15. These successive roots were then extrapolated to the limit as $m \to \infty$ (or in other words, as $N \to \infty$) by using Richardson extrapolation [15, pg. 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

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

¹The QRS treatment [14] has $s = \sin \phi_0(1)$ in those authors' notation [14, p. 6].

²By "extreme precision" is meant, in the spirit of previous papers such as [3], that "enough digits for detection" are obtained. In modern times, this means hundreds or thousands of digits, depending on the scope-of-search.

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 (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:

$$c_1 \approx 0.6054436571967327494789228424472074752208996.$$
 (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 online Inverse Symbolic Calculator tool, which is available at http://oldweb.cecm.sfu.ca/projects/ISC/ISCmain.html. 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

$$\mathcal{P}_N(s) := \sum_{k=0}^M \left(2\sqrt{1 - s^2(1 - 2k/M)^2} - \frac{1}{\sqrt{1 - s^2(1 - 2k/M)^2}} \right). \tag{4}$$

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 expansion³

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

with the coefficients d_j being absolute constants. The establishment of this form leads immediately to an historical QRS expansion

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

with corresponding absolute constants c_i , so with

$$c_1 = d_1$$

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

$$c_2 = d_1 - d_1^2 + d_2,$$

 $c_3 = d_1 - 2d_1^2 + d_1^3 - 2d_2 - 2d_1d_2 + d_3,$

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 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. **QED**

To further facilitate asymptotic analysis, we shall establish a reasonably tight bound on the unique zero s_N of Lemma 1. We shall use an elementary form of the Euler-Maclaurin summation formula valid for any continuously-differentiable function f on real interval (a, b) [2, pg. 285][16, (2.1.2)]; namely, denoting by $W(x) := x - \lfloor x \rfloor - 1/2$ the antisymmetric-sawtooth function, we have

$$\sum_{a < k \le b} f(k) = \int_a^b f(x) \, dx + \int_a^b W(x) f'(x) \, dx + W(a) f(a) - W(b) f(b). \tag{5}$$

The bounding scheme we have in mind runs as follows:

³We 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.

Lemma 2 For positive integer M := N - 1, the real, positive zero s_N satisfies

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

also

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

Remark. 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 (0, 28/27].

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

$$\mathcal{P}_N(s) = -\delta_{M, \text{ even }} + 2\sum_{k=0}^T \left(2\sqrt{1 - s^2(1 - 2k/M)^2} - \frac{1}{\sqrt{1 - s^2(1 - 2k/M)^2}}\right).$$
 (6)

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 (5), 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,

$$\mathcal{P}_N(s) > -1 + 4\sqrt{1 - s^2} - \frac{2}{\sqrt{1 - s^2}} + M\sqrt{1 - s^2}.$$
 (7)

A zero of the right-hand side of (7) 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 - (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, to explore tighter theoretical bounds, say via Euler–Maclaurin formulae 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

$$\sum_{k \in \mathbb{Z}} f(k) = \sum_{n \in \mathbb{Z}} \int_{-\infty}^{\infty} f(x)e^{2\pi i nx} dx.$$
 (8)

This holds for any Lebesgue integrable function, [6, Thm 2.12]. Generally speaking, if the left-hand sum is, as in our case for Q, to be truncated at finite limits, then we may use the relation

$$\sum_{k=0}^{M} f(k) = \sum_{n \in \mathbb{Z}} \int_{-\eta}^{M+\eta} f(x)e^{2\pi i nx} dx,$$
 (9)

provided $\eta \in (0, 1)$. This "truncated" Poisson expansion can be proved directly—e.g. via standard techniques such as summation formulae. One may establish the Poisson transformation, for example, by using (5) and integrating by parts, employing at a key step a Fourier series for the sawtooth function W [16, (2.1.7)]. Any integrable ($f \in L_1$) function with finite-interval support allows the transformation—or by applying (8) to f restricted to $[-\eta, M + \eta]$.

Theorem 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

$$\mathcal{P}_N(s) = \frac{\pi M}{s} \sum_{n=1}^{\infty} (-1)^{nM} J_2\left(\frac{\pi nM}{s}\right), \tag{10}$$

where J_2 is the standard Bessel function of order 2.

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

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

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

$$\mathcal{P}_{N}(s) = \sum_{n \in \mathbb{Z}} \frac{M}{s} e^{i\pi nM} \int_{0}^{\pi} dt \left(1 - 2\sin^{2} t\right) e^{-\pi i n \frac{M}{s} \cos t}$$

$$= \frac{M}{s} \sum_{n \in \mathbb{Z}} e^{i\pi nM} \int_{0}^{\pi} \cos\left(2t\right) e^{-\pi i n \frac{M}{s} \cos t} dt$$

$$= \frac{\pi M}{s} \sum_{n=1}^{\infty} (-1)^{nM} J_{2}\left(\frac{\pi n M}{s}\right), \tag{11}$$

where the final equation (11) follows from the representation for J_2 in [1, eqn. 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

$$0 = \sum_{n=1}^{\infty} J_2 \left(\frac{\pi n M}{s_N} \right) (-1)^{nM}, \tag{12}$$

and has a proven constraint; namely, if we write

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

then $0 < \delta_N < 20/19$. 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 $\{\pi nM/s_N : n = 1, 2, 3, ...\}$ 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,

$$J_2(z) = \sqrt{\frac{2}{\pi z}} \left(\cos(z - 5\pi/4) - \frac{15}{8z} \sin(z - 5\pi/4) \right) + O\left(z^{-5/2}\right). \tag{13}$$

This kind of asymptotic is presented in most references that explain Bessel functions, say [1, p. 364]. However, if one desires *effective* bounds—that is, explicit big-O constants, the reference [5] provides a method for effective bounds (and convergent—not asymptotic—series) for $J_n(z)$, any integer n.

Compelled by the appearance of the cos-sin terms in the Bessel asymptotic (13), we define a set of offset-periodic zeta functions:

$$Q_{s}(z) := \sum_{n=1}^{\infty} \frac{\cos(\pi nz - 5\pi/4)}{n^{s}}$$

$$= -\frac{1}{\sqrt{2}} \left\{ \sum_{n=1}^{\infty} \frac{\cos(\pi nz)}{n^{s}} + \sum_{n=1}^{\infty} \frac{\sin(\pi nz)}{n^{s}} \right\}, \qquad (14)$$

$$\mathcal{R}_{s}(z) := \sum_{n=1}^{\infty} \frac{\sin(\pi nz - 5\pi/4)}{n^{s}}$$

$$= \frac{1}{\sqrt{2}} \left\{ \sum_{n=1}^{\infty} \frac{\cos(\pi nz)}{n^{s}} - \sum_{n=1}^{\infty} \frac{\sin(\pi nz)}{n^{s}} \right\}$$

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:

$$Q_s(z) = -\frac{1}{\sqrt{2}} \left(\operatorname{Re} \operatorname{Li}_s \left(e^{i\pi z} \right) + \operatorname{Im} \operatorname{Li}_s \left(e^{i\pi z} \right) \right), \tag{16}$$

$$\mathcal{R}_s(z) = \frac{1}{\sqrt{2}} \left(\operatorname{Re} \operatorname{Li}_s \left(e^{i\pi z} \right) - \operatorname{Im} \operatorname{Li}_s \left(e^{i\pi z} \right) \right). \tag{17}$$

Here $\text{Li}_s(z) := \sum_{n=0}^{\infty} z^n/n^s$ for |z| < 1 and its analytic continuation for other z [13]. $Q_s(z) = 0$ can, for example be solved with polylogarithm calculations, using the first of these two relations. Of special interest, now, is the Erdélyi expansion [10, Vol. 1, p. 29], [9]:

$$\operatorname{Li}_{s}\left(e^{i\pi z}\right) = \Gamma(1-s)(-i\pi z)^{s-1} + \sum_{m\geq 0} \frac{\zeta(s-m)}{m!}(i\pi z)^{m},$$
 (18)

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

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

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

$$Q_{1/2}(z) = -\frac{1}{\sqrt{z}} + \sum_{n \ge 0} q_n z^n, \tag{19}$$

where the coefficients enjoy a closed form

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

(An empty product is interpreted as 1.) It is fascinating that, starting with q_1 , the coefficients in (19) are alternating in sign. Indeed, an alternative series for $Q_{1/2}$ is given by

$$Q_{1/2}(z) = -\frac{1}{\sqrt{z}} - \frac{1}{\sqrt{2}} \sum_{n=0}^{\infty} \zeta(n+1/2) {2n \choose n} \left(-\frac{z}{8}\right)^n.$$
 (20)

There is another vantage point on the Q, 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 (16, 17) and a suitable reference [11, Sec 2.2] a functional relation

$$\operatorname{Li}_{s}\left(e^{i\pi z}\right) = i(2\pi)^{s-1}\Gamma(1-s)\left\{e^{-i\pi s/2}\zeta(1-s,z/2) - e^{i\pi s/2}\zeta(1-s,1-z/2)\right\}, \quad (21)$$

where now $\zeta(s,a) := \sum_{n\geq 0} 1/(n+a)^s$ is the *Hurwitz zeta function*. Formula (21) is valid for all $z\in (0,2)$, and 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 (21) has a wide scope of validity. For our present purposes the functional equation proves, for real s, via (16, 17):

Lemma 3 For real s, z with $z \in (0, 2)$ we have the following functional relations for the offset-periodic zeta functions Q, R and the Hurwitz zeta function, all entities being analytic continuations:

$$Q_s(z) = -(2\pi)^{s-1}\Gamma(1-s)\left\{\zeta(1-s,z/2)\cos((2s-1)\pi/4) + \zeta(1-s,1-z/2)\sin((2s-1)\pi/4)\right\},$$

$$\mathcal{R}_s(z) = (2\pi)^{s-1}\Gamma(1-s)\left\{\zeta(1-s,1-z/2)\cos((2s-1)\pi/4) + \zeta(1-s,z/2)\sin((2s-1)\pi/4)\right\}.$$

Note that for half-odd s such as s = -1/2, 1/2, 3/2, there is one Hurwitz zeta in play. Special instances of Lemma 3 are thus:

$$Q_{-1/2}(z) = \frac{1}{\pi\sqrt{32}} \zeta(3/2, 1 - z/2), \tag{22}$$

$$Q_{1/2}(z) = -\frac{1}{\sqrt{2}} \zeta(1/2, z/2),$$
 (23)

$$Q_{3/2}(z) = \pi \sqrt{8} \zeta(-1/2, 1 - z/2), \tag{24}$$

$$\mathcal{R}_{-1/2}(z) = -\frac{1}{\pi\sqrt{32}} \zeta(3/2, z/2), \tag{25}$$

$$\mathcal{R}_{1/2}(z) = \frac{1}{\sqrt{2}} \zeta(1/2, 1 - z/2),$$
 (26)

$$\mathcal{R}_{3/2}(z) = -\pi\sqrt{8} \zeta(-1/2, z/2). \tag{27}$$

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:

Lemma 4 (Crandall [8]) The complete analytic continuation of $\zeta(s, a)$ for $a \in (0, 1), s \neq 1 + 0i$, is given by

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

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 $s = -n \le 0$, the $\Gamma(s)$ divergence cancels a divergent m-summand, and so $\zeta(-n,a) = -B_{n+1}(a)/(n+1)$.

Though Lemma 4 was developed for computational purposes, there is one useful side result:

Corollary 1 If $s \neq 1$ be 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 always being a convergent sum).

Proof: From the relation of Lemma 4, 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. **QED**

We are now prepared to establish certain key properties of the $Q_{1/2}$ function (the reader may wish to refer to the graph, Figure 1):

Lemma 5 For z belonging to the open interval (0,2),

- 1) $Q_{1/2}(z)$ is infinitely differentiable,
- 2) $Q_{1/2}(z)$ is strictly monotone increasing,
- 3) $Q_{1/2}(z)$ has a unique zero, say $Q_{1/2}(z_0) = 0$, which z_0 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 $m \ge 0$. 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 to infer arbitrary differentiability.)

For part (2), observe that Corollary 1 assures us that the derivative of $Q_{1/2}(z) = -\zeta(1/2, z/2)/\sqrt{2}$ is positively proportional to $\zeta(3/2, z/2)$ which itself is a manifestly positive, convergent sum. Thus $Q_{1/2}$ 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,

$$Q_{1/2}(1) > -1 - \frac{\zeta(1/2)}{\sqrt{2}} + \frac{5\zeta(3/2)}{32\sqrt{2}} > 0.3.$$

(See text below for the closed form for $Q_{1/2}(1)$.) Therefore a zero-crossing exists and is unique by part (2). QED

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

Theorem 2 The sequence $\{\delta_N := M/s_N - M : M \in Z^+\}$ approaches a definite limit, said limit being the zero z_0 of Lemma 5, and so the QRS constant c_1 exists and is the unique zero of the Hurwitz zeta $\zeta(1/2, z/2)$ on $z \in (0, 2)$.

Proof: Write the Bessel asymptotic (13) as

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

then observe:

$$\sum_{n\geq 1} J_2(\pi n M/s_N) e^{i\pi n M} = \frac{1}{\pi} \sqrt{\frac{2s_N}{M}} \sum_{n\geq 1} \frac{(-1)^{nM}}{\sqrt{n}} \cos(\pi n (M+\delta_N) - 5\pi/4)$$

$$+ O\left(\frac{1}{M^{3/2}} \sum_{n\geq 1} \frac{1}{n^{3/2}}\right)$$

$$= \frac{1}{\pi} \sqrt{\frac{2s_N}{M}} \sum_{n\geq 1} \frac{1}{\sqrt{n}} \cos(\pi n \delta_N - 5\pi/4) + O\left(\frac{1}{M^{3/2}}\right).$$

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

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

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 and 5 that $\mathcal{Q}_{1/2}$ has a legitimate inverse over the entire domain $(-\infty, -\zeta(1/2)/\sqrt{2}]$, which domain containing 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 exists, namely $\lim \delta_N = z_0 = d_1 = c_1$.

 $_{
m QED}$

Using formula (16) for $Q_{1/2}$, employing also a root-finding algorithm, we produced the 1500-digit value of the zero as appears in our Appendix. We note that $Q_{1/2}(2^-) = -\zeta(1/2)/\sqrt{2} = 1.0326265761156085...$, as can be calculated by methods relevant to Lemma 3, but was also found using the *Inverse Symbolic Calculator* at

http://oldweb.cecm.sfu.ca/projects/ISC/ISCmain.html. Likewise

$$Q_{1/2}(1) = -\zeta(1/2)\left(1 - \frac{1}{\sqrt{2}}\right) = 0.42772793269397822...$$

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 (13) through the sin 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 $\zeta(1/2, z/2)$, we established a closed form for c_2 :

$$c_2 = z_0 - z_0^2 - 30 \frac{\zeta(-1/2, z_0/2)}{\zeta(3/2, z_0/2)}.$$
 (28)

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 [5]. 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 nevertheless converge absolutely.

We would like to conjecture hereby 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 2.

Finally, we also identified another constant conjectured in the Quinn-Rand-Strogatz paper [14, Equ. 55]. Therein they 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

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

appears to hold, although they admit neither having 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:

 $C \approx 2.0381693797021506217106484597282955162787140$

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,

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

$$C = \frac{1}{4} \zeta \left(\frac{3}{2}, \frac{c_1}{2} \right)$$

$$= -\frac{\partial}{\partial a} \zeta \left(\frac{1}{2}, \frac{a}{2} \right) \Big|_{a=c_1}$$
(29)

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

$$S(N,a) = -\delta_{M \text{ even}} + 2 \sum_{k=0}^{\lfloor M/2 \rfloor} \left[1 - a^2 \left(1 - \frac{2k}{M} \right)^2 \right]^{-3/2}, \tag{30}$$

where M = N - 1 as before. Now, roughly speaking (for this sketch we use " \sim " 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 (30) as

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

thus establishing (29).

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 3/2, with $\Re(s) > 1$, should be possible and surely would involve Hurwitz-zeta evaluations $\zeta(s, \cdot)$.

6 Appendix

The 42-digit extrapolation value (3) for c_1 was calculated the "quad-double" (QD) package, which is described in the paper [12] 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 datatype. While we developed this code on systems at the Lawrence Berkeley Laboratory, the final computations that produced this value, as well as that of 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 (16), we used the FindRoot[] function in *Mathematica* to obtain the following 1500-decimal-digit value for the QRS constant:

$c_1 =$

0.6054436571967327494789228424472074752208994969563226178775528774518289983516 $008468543249816966251743269169938993579021291151627795144801265809631735353064 \\ \setminus$ 584595256050633565038813531984427083311019243469327700890687316931799630146321 318600921674738308974101700798656707535895028571088566182353335405921652886974737990532059789423395594416138766678791671648224242336094997969074232060876645\ 391819722049952523384339452196056648938892980118850879743052036983141051015432 281318049205395359975228111566927152868448071109074725231099364462870585759813 556902978872565904144131678520932714670485915457952903632539044753282675876388 61626904327749455571...

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

In a similar manner, we were able to compute an extreme-precision value for the second

asymptotic coefficient c_2 , using (28) and the above value for c_1 (which equals z_0). Our result is:

 $c_2 =$

 $049956678924019508712254741131782837113318385807645036593844552606807472804809 \\ \backslash$ 193640629123367231215766692473696840868519081552791498099029321533320429423372 222519943924577142774704178956453114975865296722998849486644107032106079890568 782500057836909812999673831634689635298191481907545029851790835207345173819686\ $123307000222448421419493798532254450206713840469715701195194420211009180095272 \\ \backslash$ 144623726428767145060743241789968236338690043646356239576319389604890876316488 659231949305701716411742822220451754191278466550877434545428589049468919278630 881517355638228487397832489624269688592683645393687460149384302086483000953259\ $064265548812220671948499661345036887136145544268556752530593107400537900544405 \\ \backslash$ 596764859072509235611912060376431002707985999037345580831405988651775997745988 004892699896596361719001377875900107219982999835250170177194227551679304535912 3268797803776195706822059911091567484752687574296416395795414617268385562135696804326394277897095153735969140797904084476 ...

An extreme-precision value for the ancillary constant C is a straightforward Hurwitz-zeta computation:

C =

 $2.0381693797021506217106484597282955162787139618052080700470445643828797115246 \\ 514768685742783149625886669444341128535140447643798503409782578073167775550150 \\ 416439762723592629172346988260278224598889559085214728884733770547577308195794 \\ 504935238479223052080392621538058028555060292839643982947789392716783815030164 \\ 235812447284567463200970560145427537696364303092747566093352954489921303660334 \\ 802844081413538201842814864727350456392328724904908909642037158255780316539311 \\ 700396083119879377268429156711448843430471273241910671131491125695154365315839 \\ 268167262898466344021169327824266469648167388132014185268786770251197160205159 \\ 778357484172131134236231582561305953793108360225742011895345717913713047009900 \\ 340856947654673291245208429113901484302919893417270109446316786436540341480683 \\ 665456861781522955319022948489493525358075042761950648761778251632537541659777 \\ 136590014640121450007486011446029189620949274312909609126264640548204583785467 \\ 75797563210175228731470501519422004568794868500041268732541282751...$

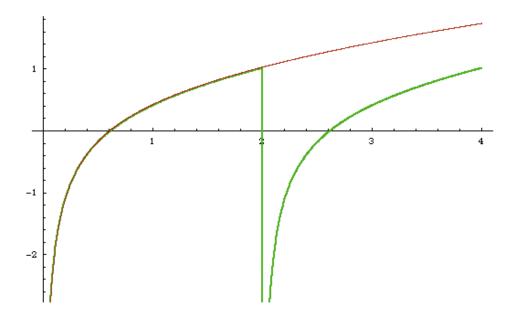


Figure 1: Plots of the offset-periodic and Hurwitz zetas $Q_{1/2}(z)$ and $-\zeta(1/2, z/2)/\sqrt{2}$, respectively (vertical) vs. z (horizontal) on (0,4). The $Q_{1/2}$ function has a discontinuity at z=2, to the left of which the two functions precisely coincide, are strictly monotone, and exhibit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

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