Supplemental material for

Quantum graphs whose spectra mimic the zeros of the Riemann zeta function

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Appendix A: The density of Riemann zeta zeros in the complex plane

Taking the logarithmic derivative $\zeta'(z)/\zeta(z)$ of the Riemann zeta function transforms its zeros into single poles in the complex plane. Therefore its real part evaluated at the critical line, $z = 1/2+\mathrm{i}t-\tau$ in the limit $\tau \to 0^-$, gives Dirac-delta peaks at all the non-trivial zeros, assuming they indeed lie on the critical line $z = 1/2 + \mathrm{i}t$. The divergent expression (2) of the Letter for the oscillating part of the density of the Riemann zeros corresponds to $\mathrm{Re}[(\zeta'/\zeta)(1/2+\mathrm{i}t)]/\pi$ using the Euler product representation of ζ and ignoring the fact that this only converges for $\mathrm{Re}\, z > 1$. Smoothing expression (2) of the Letter with a Gaussian finally makes it convergent and transforms the delta peaks into Gaussian peaks of finite width.

In order to visualize the density of Riemann zeros in the complex plane we define

$$d_{\mathbb{C}}^{\mathrm{osc}}(t+\mathrm{i}\tau) = -\frac{1}{\pi}\sum_{p}\sum_{m=1}^{\infty}\frac{\ln p}{p^{m/2}}\exp\left(-\mathrm{i}tm\ln p + \tau m\ln p\right) \tag{A1}$$

on the half plane $\tau \leq 0$ to the right of the critical line, which equals $(\zeta'/\zeta)(1/2+\mathrm{i}t-\tau)/\pi$ using the divergent series expansion of $\zeta(z)$.

To achieve convergence for $\tau \in [-1/2, 0]$, we smooth it parallel to the critical line by convolving it with a Gaussian with respect to t. For the left side $\tau > 0$ of the critical line we apply the reflection property of the ζ-function

$$\zeta(1-z) = 2(2\pi)^{-z}\cos\left(\frac{\pi z}{2}\right)\Gamma(z)\zeta(z) \tag{A2}$$

on $\zeta'/\zeta = (\ln\zeta)'$ to define

$$d_{\mathbb{C}}^{\mathrm{osc}}(t+\mathrm{i}\tau) = -[d_{\mathbb{C}}^{\mathrm{osc}}(t-\mathrm{i}\tau)]^* - 2\bar{d}_{\mathbb{C}}(t+\mathrm{i}\tau)\,, \tag{A3}$$

which relates it back to the density evaluated at $\tau < 0$ using (A1). $\bar{d}_{\mathbb{C}}$ is defined as

$$\bar{d}_{\mathbb{C}}(t+\mathrm{i}\tau) = -\frac{1}{2\pi}\ln 2\pi - \frac{1}{4}\cot\left(\frac{\pi}{4}+\frac{\pi}{2}(\mathrm{i}t-\tau)\right) + \frac{1}{2\pi}\psi\left(\frac{1}{2}-\mathrm{i}t+\tau\right)\,, \tag{A4}$$

where $\psi(z)$ denotes the digamma function [for $\tau = 0$, it corresponds to the smooth part (1) of the Letter].

Figure A1 shows the absolute value of $d_{\mathbb{C}}^{\mathrm{osc}}(t+\mathrm{i}\tau)$ with a truncation to 10000 primes and a smoothing width of 0.3, whereas Fig. A2 shows the real part of the same object. The pole-like peaks at the non-trivial Riemann zeta zeros can easily be identified.

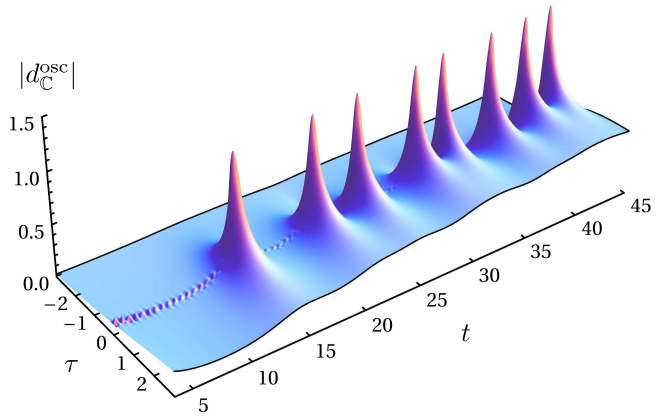

FIG. A1. Absolute value $|d_{\mathbb{C}}^{\mathrm{osc}}(t+\mathrm{i}\tau)|$. The first 10000 primes have been used and a smoothing in t-direction with a Gaussian of standard deviation 0.3 has been applied.

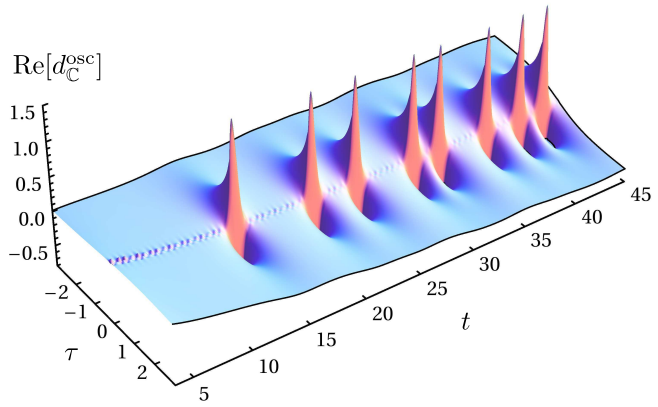

FIG. A2. Real part $\mathrm{Re}[d_{\mathbb{C}}^{\mathrm{osc}}(t+\mathrm{i}\tau)]$. The first 10000 primes have been used and a smoothing in t-direction with a Gaussian of standard deviation 0.3 has been applied.

Appendix B: Increasing the number of copies of butterfly graphs

If from the start we set the number of copies of the butterfly graphs to $l_{p,m} = m$ then the corresponding recursion

$$\cos(\theta_{p,m}) = -\frac{1}{2m^2p^{m/2}} - \sum_{d|m}^{d<m}\left(\frac{d}{m}\right)^2\cos\left(\frac{m}{d}\theta_{p,d}\right) \tag{B1}$$

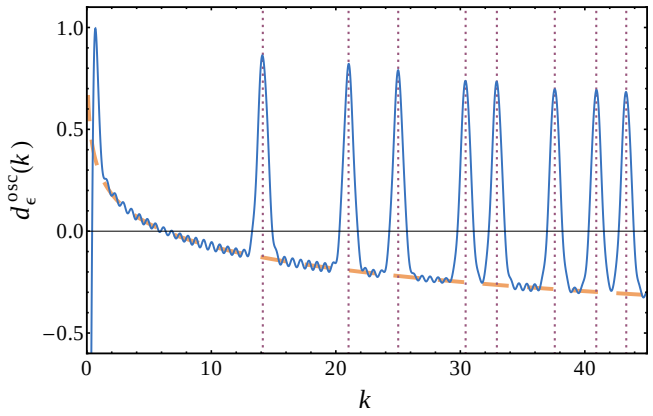

FIG. B1. Solid blue: density of exact eigenvalues of the linearly growing set of butterfly graphs (B1) smoothed with a Gaussian of width $\epsilon = 0.4$ and the mean part subtracted. The set of graphs is truncated at $\epsilon m \ln p \leq 3.7$. Dotted purple: exact zeros of the Riemann zeta function. Dashed orange: negative of the mean part of the Riemann zeros density.

is solvable with real $\theta_{p,m}$ for all (p, m) since the sum of squared divisors of m (divided by m^2) is bounded sufficiently. One can estimate

$$\sum_{d|m}^{d<m} \frac{d^2}{m^2} \leq \sum_{d|m}^{\lfloor\sqrt{m}\rfloor} \frac{d^2}{m^2} + \sum_{d|m}^{\lfloor\sqrt{m}\rfloor} \frac{1}{d^2} - 1 \tag{B2}$$
$$< \frac{1}{3\sqrt{m}} + \frac{1}{2m} + \frac{1}{6m^{3/2}} + \frac{\pi^2}{6} - 1 \equiv B(m)\,.$$

For $m \geq 4$ the bound $B(m)$ is already smaller than 1 [$B(4) = 0.957\ldots$] and the additional summand in (B1) is $1/(2m^2p^{m/2}) \leq 1/128$. Thus for all $m \geq 4$ the RHS of (B1) is smaller than 1 in absolute value. The cases $m = 1, 2, 3$ can be easily checked by direct calculation of the sum of squares of divisors. They give sufficient bounds for (B1) for the worst case $p = 2$ and hence for all primes p. Therefore, the recursion (B1) has solutions for all (p, m). Figure B1 shows the fluctuating part of the exact spectrum of a truncated set of butterfly graphs with linearly growing number of copies $l_{p,m} = m$. The enhancement of the small damped high frequency oscillations in comparison to the butterfly graphs without linear growth in Fig. 2 of the Letter is a direct consequence of the increased weight of butterflies with longer bonds.

Appendix C: Sets of butterfly graphs with identical lengths

The prescriptions (14) of the Letter and (B1) allow us to construct a sets of graphs with the same oscillating part of the density of states as the Riemann zeros, but rely on a recursive construction to find the graphs. If we

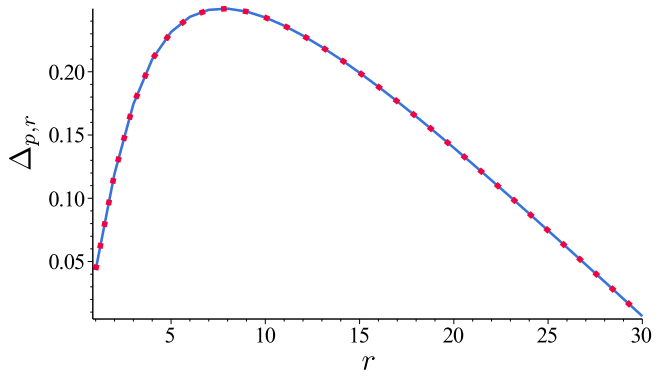

FIG. C1. Setting $p = 2$ and $R = 30$ we calculate the shift $\Delta_{2,r}$ from equally spaced angles as defined in (C11). The dotted line is from the exact numerical solution of the 30 simultaneous equations in (C4) while the solid line is derived from the approximate solutions of (C9).

perform the sum over m in Eq. (2) of the Letter to get

$$d^{\rm osc}(t) = -\frac{1}{\pi} \sum_p \ln p \frac{\sqrt{p}\cos(t \ln p) - 1}{p + 1 - 2\sqrt{p}\cos(t \ln p)}\,, \tag{C1}$$

the resultant terms

$$d_p^{\rm osc}(k) = -\frac{\ln p}{\pi} \frac{\sqrt{p}\cos(k \ln p) - 1}{p + 1 - 2\sqrt{p}\cos(k \ln p)} \tag{C2}$$

are periodic with period $2\pi/\ln(p)$. This is the same period as the solutions with $m = 1$ before. A butterfly graph of bond length $\ln(p)$ contributes to $d^{\rm osc}(k)$ with this period (and also all fractions of it; the amplitudes of all the harmonics are determined by the scattering matrix). Thus a set of butterfly graphs, all with bond length $\ln(p)$ could be constructed in a way that together they produce the correct Fourier coefficients of $d_p^{\rm osc}(k)$. We can try to find this set of butterfly graphs for each prime p so that together they again give Eq. (2) of the Letter. If we label the scattering matrices of all the butterflies $S_{p,r}$, they have to fulfill the equations

$$\sum_r \mathrm{Tr}\, S_{p,r}^m = -\frac{1}{p^{m/2}}\,, \tag{C3}$$

or

$$2\sum_r \cos(m\theta_{p,r}) = -\frac{1}{p^{m/2}}\,, \tag{C4}$$

in terms of the positive $\theta_{p,r} < \pi$.

1. Approximate solution

With a finite set of graphs $r = 1, \ldots, R$ we can find numerical solutions for the first R equations for m in (C4), but more importantly we can find approximate solutions

for any number of graphs. Assume our discrete pairs of solutions $-\pi < \pm\theta_{p,r} < \pi$ follow a density $\psi_p(\theta)$ then the limit of infinite solutions would be

$$2\int_0^\pi \cos(m\theta)\psi_p(\theta)\mathrm{d}\theta = -\frac{1}{p^{m/2}} \tag{C5}$$

for each m. Solving for ψ_p is just taking the Fourier series so

$$\pi\psi_p(\theta) = -\sum_m \frac{\cos(m\theta)}{p^{m/2}} = \frac{1-\sqrt{p}\cos(\theta)}{p+1-2\sqrt{p}\cos(\theta)}\,, \tag{C6}$$

exactly mimicking (C1).

With R pairs of θ solutions, the overall density should be $\psi_p(\theta)+R/\pi$ and we want discrete solutions that best approximate this density. Dividing the overall density between $\theta=-\pi$ and $\theta=\pi$ into $2R$ bars of equal (unit) area, we could expect to find a solution inside each bar and we approximate by placing it at the center of mass. Equivalently we are dividing the cumulative function evenly. From the symmetry, we only need to look at the solutions between 0 and π which should then satisfy

$$r-\frac{1}{2} = \frac{R\theta_{p,r}}{\pi} + \int_0^{\theta_{p,r}} \psi_p(\theta)\mathrm{d}\theta\,, \tag{C7}$$

with

$$\begin{aligned}\pi\int_0^{\theta_{p,r}} \psi_p(\theta)\mathrm{d}\theta &= -\operatorname{Im}\sum_{m=1}^{\infty}\frac{\mathrm{e}^{\mathrm{i}m\theta_{p,r}}}{mp^{m/2}}\\ &= \operatorname{Im}\left[\ln\left(1-p^{-1/2}\mathrm{e}^{\mathrm{i}\theta_{p,r}}\right)\right].\end{aligned} \tag{C8}$$

Since the argument of the logarithm in (C8) always lies in the right half plane of $\mathbb{C}$, we can write

$$\pi r - \frac{\pi}{2} = R\theta_{p,r} + \arctan\frac{\sin\theta_{p,r}}{\cos\theta_{p,r}-\sqrt{p}}\,, \tag{C9}$$

or equivalently

$$\tan(\pi\Delta_{p,r}) = \frac{\sin\theta_{p,r}}{\sqrt{p}-\cos\theta_{p,r}}\,, \tag{C10}$$

with $-1/2<\Delta_{p,r}<1/2$, where we defined the shift from equally spaced angles as

$$\Delta_{p,r} = \frac{R\theta_{p,r}}{\pi} - r + \frac{1}{2}\,. \tag{C11}$$

2. Examples

For $R=30$ we plot the shifts (C11) for $p=2$ for both the exact solutions of the 30 equations in (C4) as well as the approximate solutions from (C9) or (C10) in Fig. C1. At the level of the accuracy visible in the graph, these shifts are essentially identical.

Taking a larger number of approximate solutions by setting $R=100$ we place a Gaussian smoothed delta function (of width $\epsilon=\pi/10$) on each of the $\pm\theta_{2,r}$ and their periodic repetitions and subtract the mean part $100/\pi$. Plotting the result as the solid line in Fig. C2 we can compare to the (equally smoothed) $p=2$ term of (C1). In terms of angles $\theta=k\ln(2)$ this is just the convolution of $\psi_2(\theta)$ with the same Gaussian and we overlay this result as a dotted line in Fig. C2. Again the lines are indistinguishable in the graph.

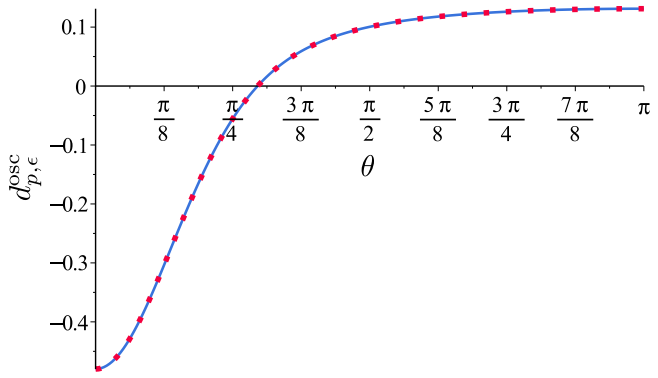

FIG. C2. The solid line is the density of states of 100 butterfly graphs of length ln(2) smoothed by a Gaussian function of width $w=\pi/10$ and with the mean part $100/\pi$ subtracted. The dotted line instead is the $p=2$ term of Eq. (C1) of the Letter, transformed to $\theta=k\ln(2)$ and smoothed with the same Gaussian.

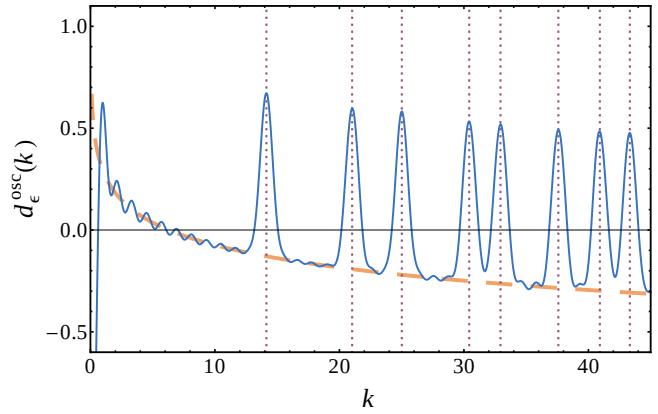

FIG. C3. Solid blue: density of eigenvalues of the set of butterfly graphs involving identical bond lengths for each prime up to $p=181$ derived using (C10) and the low value of $R=10$. The result is smoothed with a Gaussian of width $\epsilon=0.5$ and the mean part has been subtracted. Dotted purple: exact zeros of the Riemann zeta function. Dashed orange: negative of the smooth part of the Riemann zeros density.

Even a small set of graphs is enough to be able to pick out the zeros of the Riemann zeta function. Setting $R=10$ for example, we plot in Fig. C3 the smoothed oscillating part $d^{\mathrm{osc}}_{\epsilon}(k)$ of a complete set of butterfly graphs with equal bond lengths $\ln(p)$ for primes up to 181. The spectrum corresponds to the approximate solutions using (C10).