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Phys. Rev. Lett. **107**, 100201 — Published 29 August 2011

DOI: 10.1103/PhysRevLett.107.100201

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The Hilbert–Pólya conjecture states that the imaginary parts of the zeros of the Riemann zeta function are eigenvalues of a quantum hamiltonian. If so, conjectures by Katz and Sarnak put this hamiltonian in Altland and Zirnbauer's universality class C. This implies that the system must have a nonclassical two-valued degree of freedom. In such a system, the dominant primitive periodic orbits contribute to the density of states with a phase factor of -1. This resolves a previously mysterious sign problem with the oscillatory contributions to the density of the Riemann zeros.

PACS numbers: 02.10.De 05.45.-a 03.65.Sq

The distribution of prime numbers among the integers is a fundamental problem of number theory (see e.g. [1]). It is closely connected to the properties of Dirichlet L functions (including the Riemann zeta function), defined via

$$L(s,\chi) := \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s} \tag{1}$$

for $\mathrm{Re}\, s > 1$ and by analytic continuation elsewhere, where $\chi(n)$ is a primitive Dirichlet character: $\chi(n)$ is periodic with smallest period d, has magnitude one or zero, is zero if d and n are not coprime, and obeys $\chi(mn) = \chi(m)\chi(n)$. The Riemann zeta function is given by $\zeta(s) := L(s,1)$. According to the *generalized Riemann hypothesis*, any zero of $L(s,\chi)$ with $0 < \mathrm{Re}\, s < 1$ is on the *critical line* $\mathrm{Re}\, s = \frac{1}{2}$; these are the *nontrivial zeros*, which we will write as $\rho_k = \frac{1}{2} + i\gamma_k$. The generalized Riemann hypothesis implies that each γ_k is real, and this in turn can be shown to imply that the number of primes less than x in the arithmetic progression $a, a+d, a+2d, \ldots$ (with a less than and coprime to d) is, in the limit of large x,

$$\pi_{a,d}(x) = \frac{1}{\varphi(d)}\mathrm{Li}(x) + O(x^{1/2+\epsilon}) \tag{2}$$

for all $\epsilon > 0$, where $\varphi(d)$ is the number of integers less than and coprime to d (the Euler totient function), and $\mathrm{Li}(x)$ is the logarithmic integral function. The exponent of x in the error term increases to $\frac{1}{2} + \max \mathrm{Im}\, \gamma_k + \epsilon$ if the generalized Riemann hypothesis is false.

It is an old idea, now generally known as the *Hilbert–Pólya conjecture* (see [2] for a historical review), that the nontrivial zeros of each L function are the eigenvalues of an operator (on some Hilbert space) that takes the form $\frac{1}{2} + iH$, where H is self-adjoint; each L function would have a different H. Furthermore, $L(\frac{1}{2} + iE, \chi)$ is conjectured to be proportional to the spectral determinant $\det(E - H)$; since the eigenvalues of a hermitian operator must be real, the Hilbert–Pólya conjecture implies the generalized Riemann hypothesis. An explicit construction of the H's for the different L functions (or, less ambitiously, just for the Riemann zeta function) would therefore be extremely important.

A large body of analytic and numerical work strongly supports the *Montgomery–Odlyzko law* (see e.g. [3]), which states that the statistical distribution of the γ_k's for each L function is the same as the Wigner–Dyson distribution of the eigenvalues of large hermitian matrices with real diagonal entries and complex off-diagonal entries, each selected from a gaussian distribution; this is the *gaussian unitary ensemble* (GUE) [4]. A large body of analytic and numerical work also strongly supports the *Bohigas–Giannoni–Schmit conjecture* [5], which states that the energy eigenvalues of the hamiltonian for a system that is classically chaotic, and not time-reversal invariant, also obey the GUE distribution. This leads to the *generalized Berry conjecture* [6]: the operator H for each L function can be obtained by quantizing a classically chaotic system that is not time-reversal invariant.

Katz and Sarnak [7] have conjectured that L functions corresponding to Dirichlet characters that are real $[\chi(n) = 0, \pm 1]$ and even $[\chi(-1) = +1]$ form a "family" (that includes the Riemann zeta function) whose members are related (in some fashion) by a symplectic symmetry, and furthermore that the spacings of the γ_k's for each member of this family is governed by the distribution of eigenphases of random unitary symplectic matrices. This agrees with the GUE distribution for $\gamma_k \gg 1$, and predicts a gap in the spectrum near zero; this is well supported by numerical evidence from these L functions [7, 8]. Other proposed families have unitary or orthogonal symmetries.

Altland and Zirnbauer [9] have classified the possible symmetry classes of quantum hamiltonians. The distribution of γ_k's found by Katz and Sarnak is a predicted property of the energy eigenvalues for a chaotic system in Altland and Zirnbauer's class C. We therefore interpret the Katz–Sarnak conjecture, in the context of the Hilbert–Pólya conjecture, to mean that the quantum system corresponding to the Riemann zeta function (or any other member of its symplectic family of L functions) should have a hamiltonian in class C.

A hamiltonian in class C takes the form of a generator of $USp(N)$; more specifically,

$$H = A + \vec{\sigma}\cdot\vec{S}, \tag{3}$$

where A is a hermitian operator that (when expressed as a matrix in a suitable basis) is imaginary and antisymmetric, and each S_i ($i = 1, 2, 3$) is a hermitian operator that (when expressed as a matrix in the same basis) is real and symmetric; finally, σ_i is a Pauli matrix acting in an additional two-dimensional Hilbert space. This extra "nonclassical two-valuedness" ("klassisch nicht beschreibbare Zweideutigkeit", Pauli's [10] description of electron spin) is a previously unrecognized essential ingredient in any attempt to construct a quantum hamiltonian with eigenvalues corresponding to the imaginary parts of the nontrivial Riemann zeros.

Next, consider the "completed" zeta function $\Lambda(s) := \Gamma_\infty(s)\zeta(s)$, where $\Gamma_\infty(s) := \pi^{-s/2}\Gamma(s/2)$ and $\Gamma(z)$ is the Euler gamma function. The completed zeta function obeys Riemann's functional equation $\Lambda(s) = \Lambda(1-s)$, and is real on the critical line; the zeros of $\Lambda(s)$ coincide with the nontrivial zeros of $\zeta(s)$. It follows that the number of zeros of $\zeta(s)$ on the critical line with imaginary part between zero and $E > 0$ is given by

$$N(E) = \tfrac{1}{\pi}\,\mathrm{Im}\ln\Lambda(\tfrac{1}{2}+\epsilon+iE)+1, \tag{4}$$

where ϵ is a positive infinitesimal [11]. We can write $N(E)$ as the sum of a smooth contribution and an oscillating contribution [6]:

$$\begin{aligned} N(E) &= \overline{N}(E) + N_{\mathrm{osc}}(E), & (5)\\ \overline{N}(E) &= \tfrac{1}{\pi}\,\mathrm{Im}\ln\Gamma_\infty(\tfrac{1}{2}+iE)+1 & \\ &= \tfrac{E}{2\pi}\ln\big(\tfrac{E}{2\pi}\big) - \tfrac{E}{2\pi} + \tfrac{7}{8} + O(E^{-1}), & (6)\\ N_{\mathrm{osc}}(E) &= \tfrac{1}{\pi}\,\mathrm{Im}\ln\zeta(\tfrac{1}{2}+\epsilon+iE). & (7) \end{aligned}$$

Using the Euler product formula $\zeta(s) = \prod_p (1-p^{-s})^{-1}$, where p is a prime, we get the formal expression

$$\begin{aligned} N_{\mathrm{osc}}(E) &= -\frac{1}{\pi}\,\mathrm{Im}\sum_p \ln(1-p^{-(1/2+iE)}) \\ &= +\frac{1}{\pi}\,\mathrm{Im}\sum_p\sum_{r=1}^{\infty}\frac{p^{-r(1/2+iE/2)}}{r} \\ &= -\frac{1}{\pi}\sum_p\sum_{r=1}^{\infty}\frac{\sin(rE\ln p)}{r\,p^{r/2}}. \end{aligned} \tag{8}$$

This expression is formal because the Euler product does not converge on the critical line. Its value is in its similarity to the corresponding expression for the number of energy eigenvalues less than E of a hamiltonian for a classically chaotic system whose classical periodic orbits are all isolated and unstable. For a system without the two-valued quantum degree of freedom required by class C, the smooth contribution is given by the Weyl formula (see e.g. [12])

$$\overline{N}(E) = \int \frac{d^f x\, d^f p}{(2\pi\hbar)^f}\,\Theta(0<h(x,p)<E), \tag{9}$$

where $\Theta(S) = 1$ if S is true and 0 if S is false, f is the number of classical degrees of freedom, and $h(x,p)$ is the classical hamiltonian [13]. The oscillating contribution is given by a formal sum over primitive periodic orbits (labelled by po) and their repetitions (labelled by r),

$$N_{\mathrm{osc}}(E) = +\frac{1}{\pi\hbar}\sum_{po}\sum_{r=1}^{\infty}\frac{\sin(rS_{po}/\hbar - r\mu_{po})}{r\,|\det(M_{po}^r - I)|^{1/2}}, \tag{10}$$

where the primitive orbit has action $S_{po}(E)$, Maslov phase $\mu_{po}(E)$, and stability matrix $M_{po}(E)$.

If we hypothesize a dynamical system in which the primitive periodic orbits are labelled by prime numbers [6], then Eq. (10) bears a strong resemblance to Eq. (8). However, there are two well known problems with getting Eq. (10) to reproduce Eq. (8) precisely [6]. First, $|\det(M_{po}^r - I)|$ generically does not have the form of a simple exponential like p^r. Second, no value of μ_{po} in Eq. (10) will result in the overall minus sign on the right-hand side of Eq. (8).

The generalization of Eq. (10) to class C has been considered by Gnutzmann et al [14]. As a prototypical class-C system, they studied a Fermi sea of electrons (with the Fermi surface at $E = 0$) in a hard-wall billiard in a strong magnetic field (to break time-reversal invariance). There are then both electron and hole excitations, and σ_3 is defined to be $+1$ for electrons and -1 for holes. Part of the billiard boundary is superconducting, and this leads to Andreev reflection: when hitting the superconducting boundary, an electron turns into a hole (and vice versa) and "retroflects", initially retracing the incoming path. There is an extra phase factor of $-i$ for each Andreev reflection, in addition to the Maslov phase. In general, the action of a primitive periodic orbit takes the form [14]

$$S_{po}(E) = S_{po}^{(e)}(E) + S_{po}^{(h)}(E), \tag{11}$$

where $S_{po}^{(e)}(E)$ $[S_{po}^{(h)}(E)]$ is the action of those segments of the orbit where the excitation is an electron [hole]. For a given segment,

$$S_{\mathrm{seg}}^{(h)}(E) = -S_{\mathrm{seg}}^{(e)}(-E). \tag{12}$$

Gnutzmann et al show that the dominant periodic orbits are *self-dual*. A self-dual orbit includes an odd number N_A of Andreev reflections, and is traced twice, with each segment traced once as an electron and once as a hole. For a self-dual orbit, we therefore have

$$S_{po}(E) = S_{po}^{(e)}(E) - S_{po}^{(e)}(-E) \simeq E\tau_{po}, \tag{13}$$

where $\tau_{po} = 2\,\partial S_{po}^{(e)}/\partial E$ is the period of the complete twice-traced orbit. The Maslov phases of the two tracings cancel, but the factor of $-i$ for each Andreev reflection results in an extra overall factor of $(-i)^{2N_A r} = (-1)^r$, where r is the number of repetitions of the complete orbit. Finally, there are two factors of the inverse square-root of the stability determinant, one for each single tracing.

The final result is therefore [14, 15]

$$N_{\rm osc}(E) = \frac{1}{\pi\hbar}\sum_{po}\sum_{r=1}^{\infty}\frac{(-1)^r\sin(rE\tau_{po}/\hbar)}{r\,|\det(M_{po}^r - I)|}. \quad (14)$$

Eq. (14) bears a much stronger resemblance to Eq. (8) for the Riemann zeros than does Eq. (10). The dominant orbit actions are linear in E, and the primitive orbits contribute with the correct sign.

We can improve the agreement if we hypothesize that the underlying dynamical system has primitive periodic orbits that are labelled by both a prime p and another integer $k = 0, 1, \ldots$ (rather than by a prime p alone), and that, for a primitive orbit so labelled, $\tau_{po} = 2^k \ln p$ and $|\det(M_{po}^r - I)| = \exp(r\tau_{po}/2)$ [16]. With this ansatz, we have (setting $\hbar = 1$)

$$\begin{aligned} N_{\rm osc}(E) &= \frac{1}{\pi}\sum_{po}\sum_{r=1}^{\infty}\frac{(-1)^r\sin(rE\tau_{po})}{r\,|\det(M_{po}^r - I)|} \\ &= \frac{1}{\pi}\sum_{p}\sum_{k=0}^{\infty}\sum_{r=1}^{\infty}\frac{(-1)^r}{r}\frac{\sin(2^k rE\ln p)}{\exp(2^k r\ln p/2)}. \end{aligned} \quad (15)$$

We now use the mathematical identity [17]

$$\sum_{k=0}^{\infty}\sum_{r=1}^{\infty}\frac{(-1)^r}{r}f(2^k r) = -\sum_{r=1}^{\infty}\frac{1}{r}f(r). \quad (16)$$

Thus Eq. (15) becomes

$$N_{\rm osc}(E) = -\frac{1}{\pi}\sum_{p}\sum_{r=1}^{\infty}\frac{1}{r}\frac{\sin(rE\ln p)}{\exp(r\ln p/2)}, \quad (17)$$

which matches Eq. (8) precisely. Thus, while the even repetitions contribute with the wrong sign in Eq. (14), these contributions can in principle be balanced (in a class-C system) by correct-sign contributions from other primitive orbits.

Next we consider our results in comparison with some earlier work.

Connes [18] has suggested that the minus sign in Eq. (8) should be explained by having the Riemann zeros be *missing* eigenvalues in an otherwise continuous spectrum of an appropriate hamiltonian H. This would explain why all repetitions contribute with the same sign, but leaves open the fundamental problem that matching Riemann zeros to missing eigenvalues does not allow for a potential proof of the Riemann hypothesis by demonstrating that $\zeta(\frac{1}{2} + iE) \propto \det(E - H)$. Instead, Connes shows that the Riemann hypothesis is equivalent to a certain trace formula for a hamiltonian with the desired continuous spectrum. In the present work, we have provided an alternative explanation for the sign discrepancy that still allows for the original formulation of the Hilbert–Pólya conjecture.

Berry and Keating [19] have suggested that the quantum hamiltonian H corresponding to the Riemann zeta function should take the form of some quantization, on some compactified phase space for one degree of freedom, of the classical hamiltonian $h(x,p) = xp$. Here we note that this hamiltonian would be in class D. To see this, consider the simplest hermitian quantization on an uncompactified phase space, $H = \frac{1}{2}(XP + PX)$, where X and P are the position and momentum operators. If we take matrix elements of this hamiltonian between basis states with real position-space wave functions, we get a hamiltonian matrix of the form $H = A$, where A is imaginary and antisymmetric. This characterizes hamiltonians in class D [9]. Class-D systems have broken time-reversal invariance, and hence have eigenvalues with a statistical distribution governed by GUE. However, since a class-D system does not have the extra nonclassical two-valued degree of freedom, Eq. (10) for $N_{\rm osc}(E)$ applies, and so the generic sign discrepancy with Eq. (8) is still present.

In conclusion, the combination of the Hilbert–Pólya conjecture (that the imaginary parts of the nontrivial zeros of the Riemann zeta function are the eigenvalues of some quantum hamiltonian) with the Katz–Sarnak conjecture (that the Riemann zeta function is a member of a family of L functions related by a symplectic symmetry) implies that a hamiltonian whose eigenvalues are the imaginary parts of the Riemann zeros should reside in class C of the Altland–Zirnbauer classification scheme. This implies that the hamiltonian should incorporate a nonclassical two-valued degree of freedom. Systems in class C generically have primitive periodic orbits that contribute to the density of the Riemann zeros with the correct sign, further strengthening the argument that class C is the right arena to seach for the elusive Riemann hamiltonian.

I thank Jeffrey Stopple for discussions and Sven Gnutzmann, Jon Keating, and Michael Berry for helpful correspondence. This work was supported in part by the National Science Foundation under grant PHY07-57035.

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[11] For small z, $\Lambda(\frac{1}{2}+z) = -c_1 - c_2 z^2 + O(z^4)$, where c_1 and c_2 are positive real constants. We choose the branch of the logarithm such that $\mathrm{Im}\ln\Lambda(\frac{1}{2}+\epsilon+iE) = -\pi$ for small positive E. As E increases, this function jumps by $+\pi$ whenever $\Lambda(\frac{1}{2}+iE)$ changes sign.

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[13] For a class-C system, $h(x,p)$ is replaced in the Weyl formula by $a(x,p) + |\vec{s}(x,p)|$, where $a(x,p)$ and $s_i(x,p)$ are the classical formulations of the operators A and S_i.

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[15] Note that orbit repetitions were not included in the formulae of ref. [14], since primitive orbits are expected to dominate (S. Gnutzmann, private communication).

[16] As noted earlier, $|\det(M_{po}^r - I)|$ does not generically have this simple exponential dependence on r. This issue does not appear to be ameliorated solely by having H be in class C, and so instead should emerge as a detailed property of the correct class-C system.

[17] To verify Eq. (16), set $n = 2^k r$, and consider the terms on the left-hand side with a fixed value of n. The possible values of r are then $n, n/2, \ldots, n/2^m$, where 2^m is the largest power of 2 that divides n. Only the last of these possible values of r is odd. Summing $(-1)^r/r$ over this set thus yields $(1/n)(1+2+\ldots+2^{m-1}-2^m) = -1/n$. The remaining sum over n is now the same as the sum over r on the right-hand side of Eq. (16).

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