$H = xp$ Model Revisited and the Riemann Zeros

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Berry and Keating conjectured that the classical Hamiltonian $H = xp$ is related to the Riemann zeros. A regularization of this model yields semiclassical energies that behave, on average, as the nontrivial zeros of the Riemann zeta function. However, the classical trajectories are not closed, rendering the model incomplete. In this Letter, we show that the Hamiltonian $H = x(p + \ell_p^2/p)$ contains closed periodic orbits, and that its spectrum coincides with the average Riemann zeros. This result is generalized to Dirichlet L functions using different self-adjoint extensions of H. We discuss the relation of our work to Polya's fake zeta function and suggest an experimental realization in terms of the Landau model.

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One of the most promising avenues to prove the Riemann hypothesis (RH) is to find a self-adjoint operator H whose spectrum contains the imaginary part of the nontrivial Riemann zeros [1,2]. This idea was suggested by Polya and Hilbert at the dawn of the twentieth century and still, one hundred years later, it remains unproved, as well as the RH itself (see [3] for a recent review on physical approaches to the RH). There are significant hints of the validity of the Polya-Hilbert conjecture. Two of them are the Montgomery-Odlyzko law, which states that the local statistics of the Riemann zeros is given by the Gaussian unitary ensemble of random matrix theory, and the formal similarities between counting formulas of *zeros* in number theory and energy levels in quantum chaotic systems. In this web of relationships, Michael Berry suggested the existence of a classical Hamiltonian whose quantum version would realize the Polya-Hilbert conjecture [4]. This conjectured Hamiltonian must satisfy the following conditions: (i) be chaotic, with isolated periodic orbits related to the prime numbers, (ii) break time reversal symmetry, to agree with the Gaussian unitary ensemble statistics, and (iii) be quasi–one dimensional. These conditions were derived from a formal analogy between the fluctuation part of the Riemann-Mangoldt formula of the zeros of the zeta function and the Gutzwiller formula for the fluctuation term of the counting of energy levels in a chaotic quantum system.

In 1999 Berry and Keating showed that the classical Hamiltonian $H_{\rm cl} = xp$ fulfills conditions (ii) and (iii) but not condition (i) [5]. The failure of (i) is dramatic because this Hamiltonian is integrable, and therefore not chaotic, and moreover the classical trajectories are not closed, which leads naturally to a continuum spectrum. Indeed, the Hamiltonian $H_{\rm cl} = xp$ can be quantized in terms of the self-adjoint operator $\hat{H} = (x\hat{p} + \hat{p}x)/2$, with $\hat{p} = -i\hbar d/dx$, and its spectrum is given by the real line [6,7]. In order to obtain a discrete spectrum, out of the xp model, Berry and Keating imposed the conditions $|x| \geq \ell_x$ and $|p| \geq \ell_p$, where the minimal length ℓ_x and minimal momentum ℓ_p span the Planck area $\ell_x \ell_p = 2\pi\hbar$ in phase space. Subject to these conditions, a particle with energy $E > 0$ describes a truncated hyperbola in phase space,

$$x(t) = \ell_x e^t, \qquad p(t) = \frac{E}{\ell_x} e^{-t}, \qquad 0 \leq t \leq T_E = \log \frac{E}{h}. \tag{1}$$

The area bounded by this trajectory, and the $x = \ell_x$ and $p = \ell_p$ axes, measured in Planck units, give the semiclassical number of states

$$N(E) = \frac{E}{2\pi\hbar}\left(\log \frac{E}{2\pi\hbar} - 1\right) + \frac{7}{8} + \ldots, \tag{2}$$

where the constant $7/8$ comes from a Maslov phase. Rather remarkably, this formula coincides with the asymptotic behavior of the average term in the Riemann-Mangoldt formula [1], where $E/\hbar$ is interpreted as the height of a nontrivial zero. Incidentally, Connes also studied the xp Hamiltonian imposing the constraints $|x| \leq \Lambda$, $|p| \leq \Lambda$, where Λ is a cutoff [8]. In the limit $\Lambda \to \infty$, one obtains semiclassically a continuum spectrum, where the smooth Riemann zeros appear as missing spectral lines. However, a more appropriate interpretation of Connes's result is that Riemann's formula gives a finite size correction to the energy levels. Connes's regularization was later derived from the Landau model of a particle moving in two dimensions (2D) under the action of external magnetic and electric fields [9].

A fundamental problem of the Berry-Keating model is that the classical trajectories are not closed. The particle starts at the phase space point $(\ell_x, E/\ell_x)$, and stops at the point $(E/\ell_p, \ell_p)$ in a time T_E [see Eq. (1)]. The xp Hamiltonian breaks time reversal, so the particle cannot return to its initial position along the time reversed path. Berry and Keating suggested different ways to close the trajectories, such as the identification of x and $-x$, and p

and $-p$, or the use of symmetries, but no definite conclusion was reached, and consequently, the connection of (2) with the Riemann formula could not be put on more solid grounds.

The aim of this Letter is to show that the closure problem can be solved by a modification of the xp model that preserves several of its features, but makes it into a consistent quantum model. First of all, we shall constrain the motion of the particle to the half line $\ell_x \le x \le \infty$ while the momentum is allowed to take any real value (see [10] for a quantum mechanical model with a Morse potential defined on the half line whose spectrum is similar to that of the regular Riemann zeros). The classical Hamiltonian is defined as

$$H_{\rm cl} = x\left(p + \frac{\ell_p^2}{p}\right), \qquad x \ge \ell_x, \qquad p \in \mathbb{R}, \tag{3}$$

where ℓ_p is a coupling constant with dimensions of momentum. If $|p| \gg \ell_p$, the extra term added to the xp Hamiltonian is negligible, but it becomes dominant if $|p| \ll \ell_p$, forbidding the particle to escape to infinity, since that would cost an infinite energy. This result is made clear by the solution of the Hamilton equations

$$\dot{x} = x\left(1 - \frac{\ell_p^2}{p^2}\right), \qquad \dot{p} = -\left(p + \frac{\ell_p^2}{p}\right), \tag{4}$$

given by

$$x(t) = \frac{\ell_x}{|p_0|} e^{2t}\sqrt{(p_0^2 + \ell_p^2)e^{-2t} - \ell_p^2}, \qquad p(t) = \pm\sqrt{(p_0^2 + \ell_p^2)e^{-2t} - \ell_p^2}. \tag{5}$$

A complete cycle of a classical trajectory can be described as follows (see Fig. 1). The particle starts at the point $A = (\ell_x, p_0)$ (with $|p_0| \ge \ell_p$). Then, x increases and p decreases monotonically reaching the turning point $B = (x_m(E), \ell_p)$, where $x_m(E) = E/2\ell_p$ is the maximal elongation. After that, the particle moves backwards to the point $C = (\ell_x, \ell_p^2/p_0)$, which is attained in a time

$$T_E = \cosh^{-1}\frac{E}{2h} \to \log\frac{E}{h} (E \gg h), \tag{6}$$

where $h \equiv \ell_x \ell_p$ should not still be identified with Planck's constant $2\pi\hbar$. At the point C, the particle bounces off, meaning that its momentum ℓ_p^2/p_0 becomes p_0, and the cycle repeats itself, with T_E being the period. The latter process preserves the total energy, and it is analogous to the change in the momentum, $p \to -p$, of a particle hitting a wall. The classical energies are bounded from below by the condition $|E| \ge E_0^{\rm cl} = 2h$. The minimum energy corresponds to the static solutions $x = \ell_x$ and $p = \pm\ell_p$.

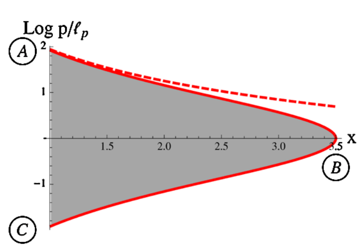

FIG. 1 (color online). Classical trajectories given in Eqs. (5) (continuous line) and (1) (dashed line).

An extra condition on the Riemann dynamics is the existence of complex periodic orbits (instantons) with periods $T_{{\rm inst},m} = \pi i m$ (with m an integer) [5]. The orbits (1) of the xp model are periodic in imaginary time, but with a wrong period $2\pi i$. After a complex time $\Delta t = i\pi$, the position and momenta change sign, which led Berry and Keating to suggest the aforementioned identification between x and $-x$, and p and $-p$, which in any case does not close the orbits. This problem does not arise for the Hamiltonian (3), which contains complex periodic orbits with a period πi, as can be seen from Eq. (5).

The semiclassical number of states is given by the phase space area swept by the particle measured in units of $2\pi\hbar$, and it is given by

$$N(E) = \frac{E}{2\pi\hbar}\left(\cosh^{-1}\frac{E}{2h} - \sqrt{1 - (2h/E)^2}\right) \simeq \frac{E}{2\pi\hbar}\left(\log\frac{E}{h} - 1\right) + O(E^{-1}), \qquad \frac{E}{2h} \gg 1. \tag{7}$$

This formula agrees with Eq. (2) if $h = 2\pi\hbar$, up to the constant term, which does not arise in (7). Let us now proceed to the quantization of the classical Hamiltonian (3). We choose the normal ordering prescription,

$$\hat{H} = x^{1/2}\left(\hat{p} + \frac{\ell_p^2}{\hat{p}}\right)x^{1/2}, \tag{8}$$

where $1/\hat{p}$ is the 1D Green function satisfying $\hat{p}\hat{p}^{-1} = \hat{p}^{-1}\hat{p} = \mathbf{1}$, and whose matrix elements are

$$\left\langle x \left| \frac{1}{\hat{p}} \right| y \right\rangle = -\frac{i}{\hbar}\theta(y - x) \tag{9}$$

with $\theta(x)$ the Heaviside step function. $\hat{H}$ acts on a wave function ψ as

$$\hat{H}\psi(x) = -ix^{1/2}\left[\hbar\frac{d}{dx}\{x^{1/2}\psi(x)\} + \ell_p^2\int_{\ell_x}^{\infty}\frac{dy}{\hbar}\theta(y - x)y^{1/2}\psi(y)\right]. \tag{10}$$

This operator is Hermitian, i.e., $\langle\psi_1|\hat{H}\psi_2\rangle = \langle\hat{H}\psi_1|\psi_2\rangle$, if both wave functions satisfy the nonlocal boundary condition

$$\hbar\ell_x^{1/2}e^{i\vartheta}\psi(\ell_x) + \ell_p\int_{\ell_x}^{\infty}dx x^{1/2}\psi(x) = 0, \tag{11}$$

where $\vartheta \in [0, 2\pi)$. To derive (11), we have assumed that $\psi(x)$ decays asymptotically faster that $x^{-1/2}$. Using Eq. (10), the Schrödinger equation $\hat{H}\psi_E = E\psi_E$ becomes an integro-differential equation which can be converted into a second order differential equation and a boundary condition. The solution of both equations yields a unique square integrable eigenfunction given by

$$\psi_E(x) = x^{(iE)/2\hbar} K_{1/2-(iE)/2\hbar}\left(\frac{\ell_p x}{\hbar}\right), \quad (12)$$

where $K_\nu(x)$ is the modified K-Bessel function (the normalization factor is not included). The asymptotic behavior of (12) is given by

$$\psi_E(x) \sim \begin{cases} x^{-1/2+(iE)/\hbar} & x \ll x_m(E) \\ x^{-1/2+(iE)/2\hbar} e^{-\ell_p x/\hbar} & x \gg x_m(E), \end{cases} \quad (13)$$

where $x_m(E)$ is the maximal length of the classical trajectory. If $x \ll x_m$ the wave function $\psi_E(x)$ behaves, up to oscillations, as the eigenfunction $x^{-1/2+(iE)/\hbar}$ of the quantum Hamiltonian $x^{1/2}\hat{p}x^{1/2}$. However, $\psi_E(x)$ drops exponentially in the classical forbidden region (see Fig. 2). The Hermiticity of $\hat{H}$ requires the eigenfunctions (12) to satisfy the boundary condition (11), which in turn provides the equation for the eigenenergies, E_n,

$$\Xi_{\hat{H}}(E) \equiv e^{-i(\vartheta/2)} K_{1/2+(iE)/(2\hbar)}\left(\frac{h}{\hbar}\right) + e^{i(\vartheta/2)} K_{1/2+(iE)/(2\hbar)}\left(\frac{h}{\hbar}\right) = 0. \quad (14)$$

All the solutions of this equation will be real, if the Hamiltonian $\hat{H}$ is not only Hermitian but also self-adjoint. To verify this property we use the von Neumann theorem: $\hat{H}$ is a self-adjoint operator if the deficiency indices n_+ and n_- coincide [11,12]. These indices are the number of linearly independent solutions of the equations $\hat{H}^\dagger \psi = \pm i\psi$. Then if $n = n_+ = n_-$, the operator $\hat{H}$ admits infinitely many self-adjoint extensions parametrized by matrices of the unitary group $U(n)$. In our case we find that $n_+ = n_- = 1$; therefore, the self-adjoint extensions correspond to a phase that can be identified with the factor $e^{i\vartheta}$ appearing in Eqs. (11) and (14). This ends the proof of the reality of all the eigenenergies E_n.

If $\vartheta = 0$, all the eigenenergies are nonvanishing and form time conjugate pairs $\{E_n, -E_n\}$ with their associated eigenfunctions being related by the time reversal transformation $\psi_{-E_n}(x) = \psi^*_{E_n}(x)$. If $\vartheta = \pi$, there is a unique state of zero energy $E_0 = 0$, and eigenfunction $\psi_{E_0}(x) \propto x^{-1/2} e^{-l_p x/\hbar}$, while the nonzero energy states again form time conjugate pairs. The ground state energies $\pm E_0$ depend strongly on ϑ and can be lower or higher than the classical value $E_0^{\rm cl}$.

To fix the value of ϑ, corresponding to the average of positive Riemann zeros, we use the asymptotic behavior of Eq. (14),

$$\Xi_{\hat{H}}(E) \simeq \left(\frac{4\pi\hbar}{h}\right)^{1/2} e^{-(\pi E)/(4\hbar)} \cos\left(\frac{E}{2\hbar}\log\frac{E}{he} - \frac{\vartheta}{2}\right), \quad (15)$$

which vanishes at

$$\frac{E}{2\pi\hbar}\log\frac{E}{he} - \frac{\vartheta}{2\pi} = n + \frac{1}{2}, \qquad n \in \mathbb{Z}. \quad (16)$$

If $h = 2\pi\hbar$ and $\vartheta = 5\pi/4$, one recovers the semiclassical estimates for $N(E)$ given in Eqs. (2) and (7). A better estimate of the average of positive Riemann zeros is obtained if $N(E)$ is a half integer [4,13], which corresponds to $\vartheta = \pi/4$ (see Fig. 3). To fit the negative Riemann zeros one has to choose $\vartheta = -\pi/4$. A simultaneous fit of both positive and negative average Riemann zeros requires a modification of the Hamiltonian (3), which will be presented elsewhere.

A confirmation of these results comes from a comparison with Polya's work on the Riemann Ξ function [14] (see also [1,2]),

$$\Xi(t) = \tfrac{1}{2}s(s-1)\pi^{-s/2}\Gamma(s/2)\zeta(s), \qquad s = \tfrac{1}{2} + it, \quad (17)$$

which is an entire and even function in t, whose zeros coincides with the nontrivial zeros of $\zeta(\frac{1}{2} + it)$. Polya made a Fourier expansion of (17) and truncated it, obtaining

$$\Xi^*(t) = 4\pi^2[K_{9/4+(it)/2}(2\pi) + K_{9/4+(it)/2}(2\pi)], \quad (18)$$

which is called Polya's *fake* zeta function, since it shares several properties with $\Xi(t)$. First of all, the zeros of $\Xi^*(t)$ and $\Xi(t)$ agree on average, as can be seen using the asymptotic expansion [2]:

$$\Xi^*(t) \sim \pi^{1/4} 2^{-5/4} t^{7/4} e^{-(\pi t)/4} \cos\left(\frac{t}{2}\log\frac{t}{2\pi e} + \frac{7\pi}{8}\right). \quad (19)$$

This expression vanishes when the argument of the cosine is $n + \frac{1}{2}$, which confirms the aforementioned rule for the average location of the positive Riemann zeros, and in turn

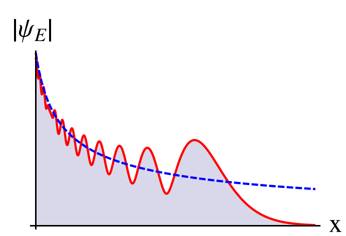

FIG. 2 (color online). Absolute value wave functions $\psi_E(x)$, given in Eq. (12) (continuous line), and $x^{-1/2+(iE)/\hbar}$ (dashed line).

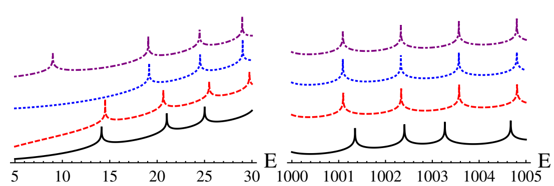

FIG. 3 (color online). From bottom to top: plot of $-\log|\Xi(E)|$ (Riemann zeros), average Riemann zeros, $-\log|\Xi_{\hat{H}}(E)|$ [eigenenergies of $\hat{H}$ for $h = 2\pi\hbar$, $\vartheta = \pi/4$], and $-\log|\Xi^*(E)|$ (Polya zeros). The cusp represents the zeros of the corresponding equations.

the choice $\vartheta = \pi/4$. A more remarkable fact is that *all* the zeros of $\Xi^*(t)$ are real, as was proved by Polya using a general theorem on entire functions [14]. This theorem can also be applied to prove the reality of all the zeros of $\Xi_{\hat{H}}(E)$, a result that we obtained using the self-adjointness of the operator $\hat{H}$.

The RH is a particular case of the generalized Riemann hypothesis, which asserts that all the nontrivial zeros of the Dirichlet $L(\chi, s)$ functions, associated to the Dirichlet character χ, lie on the critical line $\text{Re}s = \frac{1}{2}$. These functions are defined by a series and the associated Euler product ($\text{Re}s > 1$)

$$L(s, \chi) = \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s} = \prod_{p:\text{prime}} \frac{1}{1 - \chi(p)p^{-s}}, \tag{20}$$

and their analytic extension to the complex plane. $\chi(n)$ are multiplicative arithmetic functions, i.e., $\chi(nm) = \chi(n)\chi(m)$, $\chi(n + qm) = \chi(n)$, $\chi(1) = 1$, where q is the modulus of χ. L functions associated to primitive characters satisfy the functional relation [15],

$$\xi(s, \chi) = \left(\frac{\pi}{q}\right)^{-(s+a_\chi)/2} \Gamma\left(\frac{s + a_\chi}{2}\right) L(s, \chi) = \epsilon_\chi \xi(1 - s, \bar{\chi}), \tag{21}$$

where a_χ is the *parity* and ϵ_χ is the sign of a Gaussian sum,

$$a_\chi = \frac{1 - \chi(-1)}{2}, \qquad \epsilon_\chi = \frac{\tau_\chi}{i^{a_\chi} q^{1/2}}, \qquad \tau_\chi = \sum_{n=1}^{q} \chi(n) e^{(2\pi i n)/q}. \tag{22}$$

A L function is even (odd) if $a_\chi = 0(1)$. The Riemann zeta function corresponds to the trivial character $\chi(n) = 1, \forall n$, with $a_\chi = 0$, $\epsilon_\chi = 1$. Equation (21) yields the average location of the zeros of $L(\chi, s)$,

$$\frac{t}{2\pi} \log\frac{qt}{2\pi e} - \frac{1}{8} + \frac{a_\chi + \epsilon_\chi - 1}{4} = n + \frac{1}{2}, \tag{23}$$

which leads us to the following identification of parameters in the $\hat{H}$ model [see Eq. (16)],

$$\frac{E}{\hbar} = t, \quad h = \frac{2\pi\hbar}{q}, \quad \vartheta = \frac{\pi}{4}(3 - 2a_\chi - 2\epsilon_\chi). \tag{24}$$

The Riemann zeta function corresponds to the case $q = 1$, for which $h = 2\pi\hbar$, $\vartheta = \pi/4$. The correspondence (24) implies that the constant h is quantized as a function of the modulus of the L functions, attaining the classical limit, $h \to 0$, when $q \to \infty$.

A physical realization of the Hamiltonian (3) is suggested by the work of Ref. [9], which showed that $H_{\text{cl}} = xp$ emerges as the effective Hamiltonian of an electron moving in the x-y plane, subject to the action of a uniform magnetic field B, perpendicular to the plane, and an electrostatic potential $V(x, y) = V_0 xy$. If $V = 0$, the electron occupies the lowest Landau level which is completely degenerate. This degeneracy is broken by the potential $V(x, y)$, which in perturbation theory becomes the 1D Hamiltonian $H_{\text{eff}} = \omega_0 xp$, where $\omega_0 = V_0 \ell^2/\hbar$ ($\ell = \sqrt{\hbar c/eB}$ is the magnetic length). The latter Hamiltonian is obtained replacing $y \to \ell^2 p/\hbar$ in $V(x, y)$. Consider now that the particle moves in the half-plane $x \geq \ell$ and that the electrostatic potential is

$$V(x, y) = V_0 x\left(y + \frac{(2\pi\ell/q)^2}{y}\right). \tag{25}$$

Then, the effective Hamiltonian, in the lowest Landau level, in units of ω_0, becomes (3), with the identifications $\ell_x = \ell$, $\ell_p = 2\pi\hbar/q\ell$, and $h = 2\pi\hbar/q$. We expect the parameter ϑ to arise from an electric field applied at the boundary $x = \ell$ of the system.

In summary, we propose a modification of the Berry-Keating xp Hamiltonian that contains classical periodic orbits, and whose quantization agrees with the average Riemann zeros. Our results make contact with Polya's fake zeta function and we generalize them to Dirichlet L functions. Further investigation is required to incorporate the fluctuations of the Riemann zeros, providing a realization of the Polya and Hilbert conjecture.

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