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A compact hamiltonian with the same asymptotic mean spectral density as the Riemann zeros

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Abstract
For the classical hamiltonian $(x + 1/x)(p + 1/p)$, with position x and conjugate momentum p, all orbits are bounded. After a symmetrization, the corresponding quantum integral equation possesses a family of self-adjoint extensions: compact operators on the entire positive x axis, labelled by an angle α specifying the boundary condition at the origin, with a discrete spectrum of real energies E. On the cylinder $\{-\infty < E < \infty, 0 \leqslant \alpha < 2\pi\}$, there is a single eigencurve in the form of a helix winding clockwise. The rise between successive windings gets sharper as the scaled Planck's constant decreases. This behaviour can be understood semiclassically. The first two terms of the asymptotic eigenvalue density are the same as those for the density of heights of the Riemann zeros.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction: classical hamiltonian

The Riemann hypothesis [1, 2] states that all complex zeros of the Riemann zeta functions have real part 1/2, that is $\zeta(1/2 + \mathrm{i}t_n) = 0$ with t_n real. One way to prove it [1] would be to find a hermitian operator H with eigenvalues t_n. Although no such operator has been found, it has been conjectured [3, 4], by analogy with the Selberg [5, 6] and Gutzwiller [7] trace formulas, that H has a classical counterpart in the form of a hamiltonian dynamical system with some known properties. We showed [8] that the classical hamiltonian $H = xp$ has several features suggesting a relation to $\zeta(s)$. But the analogy is defective in a number of ways, one of which is that xp is not compact so there seems no natural way in which it can be quantized to yield discrete eigenvalues. See [9] for a connection between xp and the lowest Landau level of a charged particle on a planar surface in a certain electromagnetic field.

In a recent study [10] it was shown that $H = x(p + 1/p)$ can be consistently quantized and has a discrete spectrum. However, this not only spoils the symmetry in x and p but has the deficiency, shared with $H = xp$, that quantization requires regularization by an ad hoc cutoff

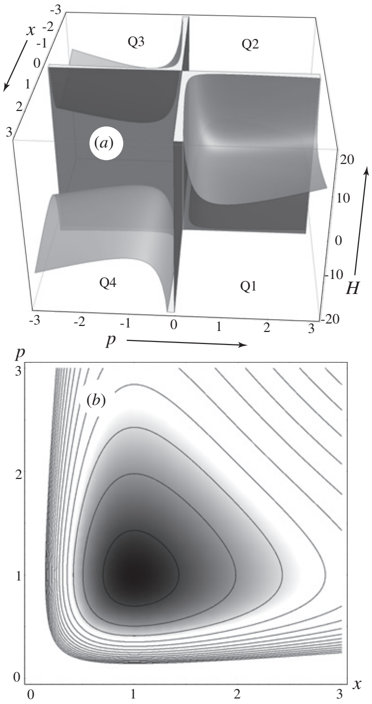

Figure 1. (*a*) 3D plot of hamiltonian $H(x, p)$ (1.3), with quadrants labelled Q. (*b*) Shaded contour plot of $H(x, p)$ in first quadrant, with light representing high and dark low.

of the x axis, involving Planck's constant. Here we explore a variant that is symmetric in x and p and for which quantization follows naturally, without cutoff. This is

$$H' = \frac{1}{T}\left(x' + \frac{l_x^2}{x'}\right)\left(p' + \frac{l_p^2}{p'}\right), \tag{1.1}$$

which, by the natural scaling

$$x' = l_x x, \qquad p' = l_p p, \qquad H' = \frac{l_x l_p}{T} H, \tag{1.2}$$

can immediately be written in the canonical form

$$H\,(x, p) = \left(x + \frac{1}{x}\right)\left(p + \frac{1}{p}\right). \tag{1.3}$$

In this classical system with one degree of freedom, orbits in the phase space x, p are contour lines of $H(x, p)$. As can be seen from figure 1, these are closed curves (unlike the hyperbolic contours of xp), so orbits are bounded. The surface has extrema (minima in the quadrants Q1, Q3, and maxima in Q2, Q4) at $|x| = |p| = 1$, with energy $|E| = 4$. A short calculation gives the area enclosed by the orbit with energy $H = E$ as

$$\begin{aligned} A(E) &= \iint_{x\geqslant 0,\, p\geqslant 0} \mathrm{d}x\,\mathrm{d}p\,\Theta(E - H(x, p)) = E\left(\mathrm{K}\left(1 - \frac{16}{E^2}\right) - \mathrm{E}\left(1 - \frac{16}{E^2}\right)\right) \\ &\underset{E\gg 0}{\rightarrow} E(\log E - 1) - \frac{4\log E}{E} + \cdots, \end{aligned} \tag{1.4}$$

where E and K denote elliptic integrals (in the notation of Mathematica [11]). On the simplest semiclassical theory, eigenvalues correspond to energies whose areas, in unscaled variables, are quantized in half-odd multiples of Planck's constant. With the natural dimensionless semiclassical parameter

$$\eta = \frac{\hbar}{l_x l_p}, \tag{1.5}$$

the quantization condition based on (1.4), giving approximate energy levels E_n, is

$$A\left(E_n\right) \approx E_n\left(\log E_n - 1\right) = 2\pi\left(n + \tfrac{1}{2}\right)\eta. \tag{1.6}$$

Up to these first two terms (E_n and $\log E_n$), this has the same form as the asymptotic formula for the heights of the Riemann zeros [1]. We will examine this connection further in section 5, after a detailed study of the quantum counterpart of (1.3) (section 2), some numerical explorations (section 3), and a semiclassical calculation (section 4) showing how (1.6) emerges as an approximation.

2. Quantum hamiltonian

With x and p now denoting operators, we seek a hermitian hamiltonian operator H, whose classical counterpart is (1.3), acting on states $|\psi\rangle$. As in [10], we choose the ordering corresponding to the Schrödinger equation

$$H\left|\psi\right\rangle = \sqrt{x + \frac{1}{x}}\left(p + \frac{1}{p}\right)\sqrt{x + \frac{1}{x}}\left|\psi\right\rangle = E\left|\psi\right\rangle. \tag{2.1}$$

This seems unsymmetrical in x and p, but it is easy to show that if x and p are interchanged the argument to follow gives the same eigenvalues. (We do not consider more general orderings, such as

$$H = \left(\left(x + \frac{1}{x}\right)^{1/2N}\left(p + \frac{1}{p}\right)^{1/N}\left(x + \frac{1}{x}\right)^{1/2N}\right)^{N}, \tag{2.2}$$

in which the special case $N = 1$ corresponds to (2.1) and the limit $N \to \infty$ (suggested by J H Hannay) seems especially interesting.)

To obtain well-defined hermitian operators corresponding to (2.1), we proceed in several stages. First, we define new states

$$|\phi\rangle = \sqrt{x + \frac{1}{x}}\left|\psi\right\rangle, \tag{2.3}$$

so that (2.1) becomes, after multiplying by p,

$$(p^2 + 1)|\phi\rangle = Ep\frac{x}{1 + x^2}|\phi\rangle. \tag{2.4}$$

In position representation, and with the customary interpretation

$$p = -\mathrm{i}\eta\,\partial_x, \tag{2.5}$$

this becomes the differential equation

$$\partial_x^2\phi\left(x\right) - \frac{\mathrm{i}Ex}{\eta(1 + x^2)}\partial_x\phi\left(x\right) + \left(-\frac{1}{\eta^2} - \frac{\mathrm{i}E}{\eta}\frac{(1 - x^2)}{(1 + x^2)^2}\right)\phi\left(x\right) = 0. \tag{2.6}$$

The further rescaling

$$\chi(x) = \phi(x)(1 + x^2)^{-\mathrm{i}E/4\eta}, \tag{2.7}$$

eliminates the first derivative, leading to

$$\partial_x^2 \chi(x) = \left(\frac{h(x)}{\eta^2} + \frac{\mathrm{i}g(x)}{\eta}\right)\chi(x), \tag{2.8}$$

where

$$h(x) = 1 - \frac{E^2x^2}{4(1+x^2)^2}, \qquad g(x) = \frac{E(1-x^2)}{2(1+x^2)^2}. \tag{2.9}$$

This can be transformed into the Heun equation (equation (31.2.3)) of [12]), but we have not found this identification helpful, because in published work we could not find the self-adjoint extensions and asymptotics that we need and that we describe later.

The equation (2.8) is of Schrödinger type but with the eigenvalue E and the semiclassical parameter η unconventionally placed and where the analogue of the potential is complex. Since $h(x)$ and $g(x)$ are even functions, it is tempting to seek square-integrable solutions of (2.8) on the full x axis, that is wavefunctions decaying at $x = \pm\infty$ that are even ($\chi(0) \neq 0,\ \partial_x\chi(0) = 0$) or odd ($\chi(0) = 0,\ \partial_x\chi(0) \neq 0$). But although such solutions can be found, they correspond to complex eigenvalues E and therefore to a nonhermitian H, because the 'potential' is complex. Numerical exploration and the analysis at the end of section 4 show that these energies are semiclassically exponentially close to the real E axis with $\mathrm{Im}\,E > 0$ for the even states and $\mathrm{Im}\,E < 0$ for the odd states.

Therefore we restrict attention to the half-line $x \geqslant 0$, and seek a relation between $\psi(0)$ and $\partial_x\psi(0)$ for which H is hermitian so the eigenvalues are automatically real. We use the fundamental condition for hermiticity, namely, for any two states in the space spanned by eigenvectors of H,

$$\langle\psi_1|\,H\,|\psi_2\rangle = \langle\psi_2|\,H\,|\psi_1\rangle^*. \tag{2.10}$$

In position representation, this can be written

$$\begin{aligned}\langle\psi_1|H|\psi_2\rangle &= \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}x'\psi_1^*(x)\langle x|H|x'\rangle\psi_2(x') \\ &= \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}x'\phi_1^*(x)\langle x|p + \frac{1}{p}|x'\rangle\phi_2(x'),\end{aligned} \tag{2.11}$$

in which the states ϕ are defined by (2.3).

We need to interpret the matrix element of $p + 1/p$, and the integral equation for ϕ in which it appears, corresponding to (2.4) without the multiplication by p, namely

$$\int_0^\infty \mathrm{d}x'\langle x|p + \frac{1}{p}|x'\rangle\phi(x') = E\frac{x}{1+x^2}\phi(x). \tag{2.12}$$

For p the interpretation is straightforward:

$$\langle x|p|x'\rangle = \mathrm{i}\eta\partial_{x'}\delta(x'-x). \tag{2.13}$$

For $1/p$, the only interpretation incorporating the fact that x and x' are non-negative is

$$\langle x|\frac{1}{p}|x'\rangle = -\frac{\mathrm{i}}{\eta}\Theta(x'-x), \tag{2.14}$$

where here and hereafter Θ denotes the unit step. Thus (2.12) has the explicit form

$$\eta\partial_x\phi(x) + \frac{1}{\eta}\int_x^\infty \mathrm{d}x'\phi(x') = \mathrm{i}E\frac{x}{1+x^2}\phi(x). \tag{2.15}$$

We will need the special case $x = 0$, that is

$$\partial_x\phi(0) = -\frac{1}{\eta^2}\int_0^\infty \mathrm{d}x\phi(x). \tag{2.16}$$

Now we can evaluate the matrix element (2.11):

$$\langle\psi_1|\,H\,|\psi_2\rangle = -\mathrm{i}\eta\int_0^\infty \mathrm{d}x\phi_1^*\,(x)\,\partial_x\phi_2\,(x) - \frac{\mathrm{i}}{\eta}\int_0^\infty \mathrm{d}x\phi_1^*\,(x)\int_x^\infty \mathrm{d}x'\phi_2(x'). \tag{2.17}$$

For the first term, integration by parts gives

$$\mathrm{i}\int_0^\infty \mathrm{d}x\phi_1^*\,(x)\,\partial_x\phi_2\,(x) = -\mathrm{i}\phi_1^*\,(0)\,\phi_2\,(0) - \mathrm{i}\int_0^\infty \mathrm{d}x\,\partial_x\phi_1^*\,(x)\,\phi_2\,(x)\,. \tag{2.18}$$

In the second term, exchanging the order of integration and interchanging x and x' give

$$\begin{aligned}\mathrm{i}\int_0^\infty \mathrm{d}x\phi_1^*(x)\int_x^\infty \mathrm{d}x'\phi_2(x') &= \mathrm{i}\int_0^\infty \mathrm{d}x'\phi_2(x')\int_0^{x'} \mathrm{d}x\phi_1^*(x)\\ &= \mathrm{i}\int_0^\infty \mathrm{d}x'\phi_2(x')\int_0^\infty \mathrm{d}x\phi_1^*(x)\\ &\quad - \mathrm{i}\int_0^\infty \mathrm{d}x'\phi_2(x')\int_{x'}^\infty \mathrm{d}x\phi_1^*(x).\end{aligned} \tag{2.19}$$

Thus

$$\langle\psi_1|\,H\,|\psi_2\rangle = \langle\psi_2|\,H\,|\psi_1\rangle^* + \mathrm{i}\left(\eta\phi_1^*\,(0)\,\phi_2\,(0) - \frac{1}{\eta}\int_0^\infty \mathrm{d}x\phi_1^*\,(x)\int_0^\infty \mathrm{d}x'\phi_2(x')\right). \tag{2.20}$$

The hermiticity condition (2.10) requires that the terms in brackets cancel, and so, after using the integral identity (2.16),

$$\partial_x\phi_1^*\,(0)\,\partial_x\phi_2\,(0) = \frac{1}{\eta^2}\phi_1^*\,(0)\,\phi_2\,(0)\,. \tag{2.21}$$

Realising that this must satisfied for all states, we finally arrive at the boundary condition relating the wavefunction to its derivative at the origin:

$$\frac{\partial_x\phi\,(0)}{\phi\,(0)} = \frac{\partial_x\chi\,(0)}{\chi\,(0)} = \frac{1}{\eta}\exp\,(\mathrm{i}\alpha)\,, \qquad \alpha \text{ real}. \tag{2.22}$$

(The first equality follows from the fact that (2.7), relating ϕ to χ, involves only x^2, so the boundary condition is the same for ϕ as for χ.)

This boundary condition, here derived as the condition for hermiticity and involving the entire positive x axis without any cutoff, was first guessed from numerical explorations. For each fixed E, we solved the differential equation (2.8) for different initial conditions $\chi'\,(0)\,/\,\chi\,(0) = a$, and found that for the solutions that decay as $x \to \infty$ the ratio a always lay on a circle with radius $1/\eta$ in the complex plane.

Our complex boundary condition is the counterpart of the Robin condition [13, 14] for states bound in a real potential, where the condition for hermiticity is that the ratio a is any real number. Corresponding to real a is the hermiticity angle α in (2.22). Each choice of α corresponds to a different self-adjoint extension of the formal operator represented by the differential equation (2.8). The special case $\alpha = 0$ resembles the Dirichlet condition for a potential, and $\alpha = \pi$ resembles the Neumann condition. Although (2.22) appears to be a local boundary condition, like the Robin condition, in fact it is nonlocal, because its derivation involves (2.16) which is a special case of the integral equation (2.15): alternatively stated, the condition (2.22) at $x = 0$ holds only for states decaying as $x \to \infty$. A different analogy is with the Aharonov-Bohm effect [15, 16], where the magnetic flux in quantum units also plays the role of a hermiticity parameter, in the form of an angle completing the Helmholtz equation in the plane with one point excised (physically, the location of the inaccessible flux), by specifying continuation around it.

3. Numerics

The argument of the preceding section shows that real eigenvalues of H are determined by the solutions of (2.8) and (2.9) with the boundary condition (2.22) for fixed hermiticity angle α. As we will see, the totality of spectra for all α correspond to a curve on the cylinder $\{-\infty < E < \infty, 0 \leqslant \alpha < 2\pi\}$. The eigenvalues satisfy the symmetry relation

$$\{E_n(\alpha)\} = \{-E_n(-\alpha)\} \quad (n = 0, 1, 2, \ldots). \tag{3.1}$$

It is not difficult to solve (2.8) numerically for fixed E and increasing x, starting from the boundary condition (2.22) with $\chi(0) = 1$, and searching real E to find the solutions that decay as $x \to \infty$. We note from (2.9) that the solution for large x is

$$\chi(x) \to C_+(E)\exp\left(\frac{x}{\eta}\right) + C_-(E)\exp\left(-\frac{x}{\eta}\right), \tag{3.2}$$

so the eigenenergies can be determined from

$$C_+(E) = \lim_{x\to\infty}\exp\left(-\frac{x}{\eta}\right)\chi(x) = 0. \tag{3.3}$$

The convergence is rapid, and for the spectra to be displayed it was sufficient to take $x \leqslant 30$.

Figure 2 illustrates the spectra for three values of the semiclassical parameter η. The pictures show

(i) There is a single eigencurve, spiralling up the cylinder.

(ii) The halves $E < 0$ and $E > 0$ of the cylinder are connected by a zero eigenvalue at $\alpha = \pi$. This is easily explained by noting that for $E = 0$ the exact decaying solution of (2.8) is

$$\chi_{E=0}(x) = \exp\left(-\frac{x}{\eta}\right) \Rightarrow \left(\frac{\partial_x\chi(0)}{\chi(0)}\right)_{E=0} = -\frac{1}{\eta}. \tag{3.4}$$

An analogous phenomenon is the zero eigenvalue for a particle in a box or a quantum billiard with Neumann boundary conditions.

(iii) As η gets smaller, the eigenvalues for fixed α crowd closer together for classically allowed energies $|E| > 4$, while a single eigencurve threads the classically forbidden region $|E| < 4$.

(iv) For small η, the risings between successive windings, although smooth, become increasingly rapid and are concentrated near $\alpha = \pi$.

In light of the symmetry (3.1), we will henceforth consider only $E \geqslant 0$.

4. Semiclassical theory

To get a clear understanding of the numerically computed eigencurves, we solve (2.8) asymptotically for small η, using a variant of the WKB method that accommodates the different η dependences of the terms involving h and g. This is based on the ansatz

$$\chi(x) = \exp\left(-\frac{1}{\eta}\int_0^x \mathrm{d}x_1 f(x_1)\right). \tag{4.1}$$

Thus (2.8) is equivalent to the nonlinear equation

$$f^2 - \eta\partial_x f = h + \mathrm{i}\eta g. \tag{4.2}$$

Expanding in powers of η, that is

$$f(x) = \sum_0^\infty \eta^n f_n(x), \tag{4.3}$$

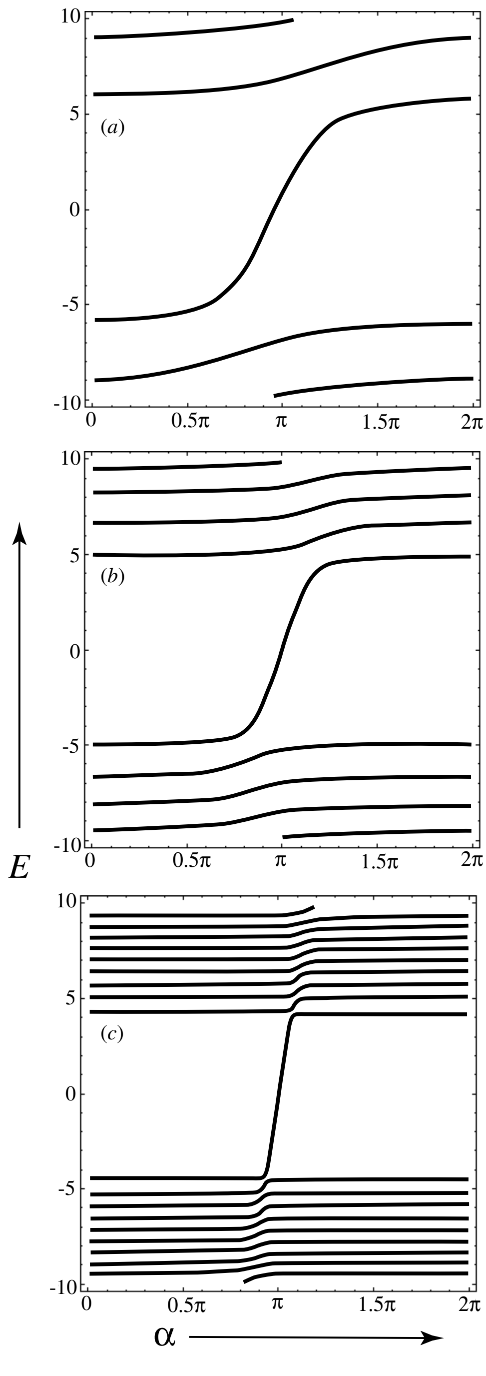

Figure 2. Eigenspirals $E(\alpha)$ on the cylinder $\{E, \alpha\}$, generated by solving equation (2.8) with the boundary condition (2.22), for semiclassical parameters (*a*) $\eta = 1$, (*b*) $\eta = 0.5$, (*c*) $\eta = 0.2$.

it is easy to find the first two terms:

$$f_0\,(x) = \sqrt{h\,(x)}, \qquad f_1\,(x) = \frac{1}{4}\partial_x \log h\,(x) + \frac{\mathrm{i}g\,(x)}{2\sqrt{h\,(x)}}. \tag{4.4}$$

Substituting into (4.1) gives the leading-order asymptotics, incorporating the terms that do not vanish as $\eta \to 0$:

$$\chi(x) \approx \frac{1}{h(x)^{1/4}} \exp\left(-\frac{1}{\eta}\int_0^x \mathrm{d}x_1 \sqrt{h(x_1)}\right) \exp\left(-\mathrm{i}\int_0^x \mathrm{d}x_1 \frac{g(x_1)}{2\sqrt{h(x_1)}}\right). \tag{4.5}$$

The two fundamental solutions of (2.8) correspond to the two signs of the square roots: to exponentially decreasing or increasing wavefunctions in the classically forbidden regions of the real axis, where $h(x)$ is positive, and oscillatory functions in the classically allowed regions, where $h(x)$ is negative.

4.1. *Eigenvalue with $0 \leqslant E < 4$*

In this case, the entire positive x axis is classically forbidden and the solution involves (4.5) with the positive square root. From (4.1) the required ratio at the origin is

$$\frac{\partial_x \chi(0)}{\chi(0)} = -\frac{f(0)}{\eta}. \tag{4.6}$$

The boundary condition (2.22) requires that $f(0)$ has modulus unity, and indeed that is what the asymptotic series solution generates; to the first few orders,

$$f(0) = \exp\left\{\tfrac{1}{4}\mathrm{i}E\eta\left(1 + \tfrac{1}{6}\eta^2(E^2-9) + \tfrac{1}{10}\eta^4(2E^4 - 30E^2 + 75) + \cdots\right)\right\}. \tag{4.7}$$

Thus the eigencurve for classically forbidden energies is, to lowest order, the straight line

$$\tfrac{1}{4}E\eta \approx \alpha - \pi \quad (0 \leqslant E < 4). \tag{4.8}$$

As figure 3 illustrates, this gets more accurate as η decreases.

4.2. *Eigenvalues with $E \geqslant 4$*

For classically allowed energies, the positive x axis consists of three regions, separated by the transition points $x_p(E)$, $x_m(E)$ where (cf. (2.9)) $h(x) = 0$:

$$x_p(E) = \tfrac{1}{4}\left(E + \sqrt{E^2 - 16}\right), \quad x_m(E) = \tfrac{1}{4}\left(E - \sqrt{E^2-16}\right) = \frac{1}{x_p(E)}. \tag{4.9}$$

The classically allowed region $x_m(E) < x < x_p(E)$ separates the forbidden regions $x > x_p(E)$ and $0 \leqslant x < x_m(E)$.

To simplify the writing of the semiclassical solution (4.5), we define

$$\phi(x_1, x_2) = \frac{1}{\eta}\int_{x_1}^{x_2} \mathrm{d}x \sqrt{h(x)}, \quad \gamma(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x \frac{g(x)}{2\sqrt{h(x)}}. \tag{4.10}$$

We will need the values of these functions involving transition points. From (2.9), we find, for the classically allowed region,

$$\begin{aligned} \phi(x_m, x_p) &= \mathrm{i}\frac{E}{2\eta}\left(\mathrm{K}\left(1 - \frac{16}{E^2}\right) - \mathrm{E}\left(1 - \frac{16}{E^2}\right)\right) = \mathrm{i}\frac{A(E)}{2\eta}, \\ \gamma(x_m, x_p) &= 0, \end{aligned} \tag{4.11}$$

in which $A(E)$ is the phase-space area (1.4) enclosed by the loop $H = E$. For the forbidden region including the origin,

$$\phi(0, x_m) = \frac{E}{8\eta}\left(\pi - 2\mathrm{E}\left(\frac{16}{E^2}\right)\right) \equiv \frac{B(E)}{\eta}, \qquad \gamma(0, x_m) = \frac{1}{4}\pi, \tag{4.12}$$

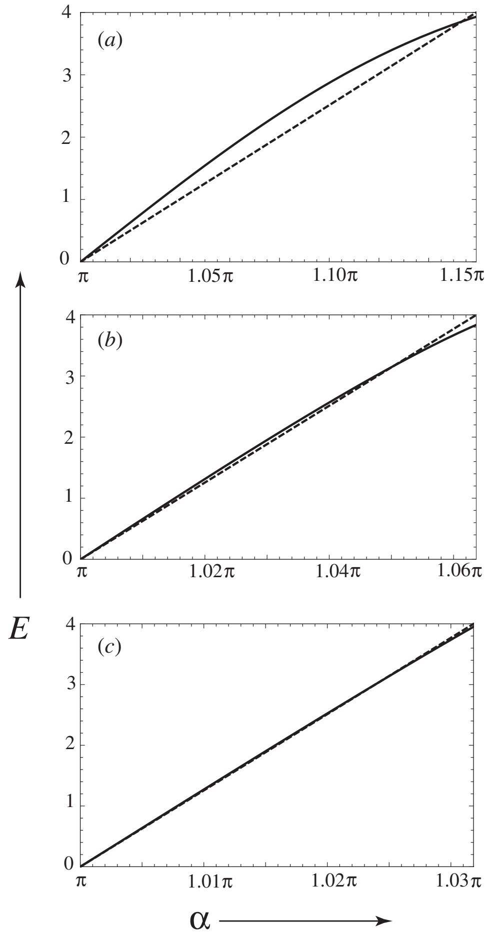

Figure 3. Lowest eigenenergy (full curves) and semiclassical approximations (4.8) (dashed curves), for (a) $\eta = 0.5$, (b) $\eta = 0.2$, (c) $\eta = 0.1$.

where $B(E)$ is the exponent governing tunnelling from the allowed region to $x = 0$:

$$B\left(E\right) = \mathrm{Im}\int_0^{x_m(E)} \mathrm{d}x p\left(x, E\right), \tag{4.13}$$

in which $p(x)$ is the complex momentum, that is, the solution of $H(x, p(x)) = E$.

In the forbidden region $x > x_p(E)$, the solution of (2.8) must decay, so

$$\chi\left(x\right) \approx \frac{1}{h(x)^{1/4}} \exp(-\phi\left(x_p, x\right)) \exp(-\mathrm{i}\gamma\left(x_p, x\right)) \quad \left(x > x_p\right). \tag{4.14}$$

To apply the boundary condition (2.22), we must follow this solution through the classically allowed region and to $x = 0$. To reach the classically allowed region, we use standard connection formulas [17–19], adapted to accommodate the additional factor involving γ,

$$\chi(x) \approx \frac{2}{|h(x)|^{1/4}} \cos\left(-\mathrm{i}\phi(x, x_p) - \frac{1}{4}\pi - \mathrm{i}\gamma(x, x_p)\right)$$
$$= \frac{2}{|h(x)|^{1/4}} \cos\left(-\mathrm{i}\phi(x_m, x) - \frac{1}{4}\pi + \mathrm{i}\phi\left(x_m, x_p\right) - \mathrm{i}\gamma(x_m, x) + \frac{1}{2}\pi\right)$$
$$(x_m < x < x_p). \tag{4.15}$$

In the second equality, we have translated the phase reference level from x_p to x_m. In the forbidden region $0 \leqslant x < x_m(E)$, the solution involves exponentially increasing as well as exponentially decreasing terms. Its determination requires a more sophisticated (and once controversial (section 13.4 of [17])) connection formula (equation (13.3.25) of [17]). But its application is straightforward, and leads to

$$\chi(x) \approx \frac{1}{h(x)^{1/4}} \cos\left(\frac{A}{2\eta}\right) \exp\left(\phi(x, x_m)\right) \exp\left(+\mathrm{i}\gamma(x, x_m)\right)$$
$$+ \frac{1}{h(x)^{1/4}} \sin\left(\frac{A}{2\eta}\right) \exp\left(-\phi(x, x_m)\right) \exp\left(-\mathrm{i}\gamma(x, x_m)\right) \quad (x < x_m). \tag{4.16}$$

Now we can apply (2.22). From (4.15), (4.11) and (4.12),

$$\chi(0) \approx \cos\left(\frac{A}{2\eta}\right) \exp\left(\frac{B}{\eta}\right) \exp\left(+\frac{1}{4}\mathrm{i}\pi\right) + \sin\left(\frac{A}{2\eta}\right) \exp\left(-\frac{B}{\eta}\right) \exp\left(-\frac{1}{4}\mathrm{i}\pi\right),$$
$$\partial_x\chi(0) \approx -\frac{1}{\eta} \exp\left(\frac{1}{4}\mathrm{i}E\eta\right) \left(\cos\left(\frac{A}{2\eta}\right) \exp\left(\frac{B}{\eta}\right) \exp\left(+\frac{1}{4}\mathrm{i}\pi\right)\right.$$
$$\left. - \sin\left(\frac{A}{2\eta}\right) \exp\left(-\frac{B}{\eta}\right) \exp\left(-\frac{1}{4}\mathrm{i}\pi\right)\right). \tag{4.17}$$

Thus the boundary condition gives the quantization rule determining the spectrum of eigenvalues E for each value of the self-adjointness parameter α:

$$\exp(\mathrm{i}\alpha) = -\exp\left(\tfrac{1}{4}\mathrm{i}E\eta\right) \frac{\left(1 + \frac{1}{2}\mathrm{i}\exp\left(-2\frac{B(E)}{\eta}\right) \tan\frac{A(E)}{2\eta}\right)}{\left(1 - \frac{1}{2}\mathrm{i}\exp\left(-2\frac{B(E)}{\eta}\right) \tan\frac{A(E)}{2\eta}\right)}. \tag{4.18}$$

As figure 4 illustrates, this reproduces the structure of the spectrum in the classically allowed region (figure 2) with increasing accuracy as η gets smaller. Two values of α are key to understanding: near $\alpha = 0$ and near $\alpha = \pi$. Then (4.18) gives the quantum conditions

$$\begin{aligned} A(E_n) &= 2\pi\left(n + \tfrac{1}{2}\right)\eta \quad \text{when} \quad \alpha = \tfrac{1}{4}E_n\eta, \\ A(E_n) &= 2\pi n\eta \quad \text{when} \quad \alpha = \pi + \tfrac{1}{4}E_n\eta. \end{aligned} \tag{4.19}$$

For most values of α, the approximation (4.18) gives eigenvalues exponentially close (and controlled by the tunnelling exponent $2B(E)/\eta$) to those given by the first of these quantum conditions, that is by the elementary semiclassical quantization rule (1.6). The rapid transition between this and the second quantum condition occurs in an interval of width $O(\eta)$ near $\alpha = \pi$,

4.3. Complex eigenvalues for the even and odd states

We can choose to regard (2.8) as a differential equation on the entire x axis. Since the functions $h(x)$ and $g(x)$ in (2.9) are even, we do not impose the hermitian boundary condition (2.22). Instead, we seek the square-integrable eigenstates are even or odd functions of x. Then the operator is nonhermitian and its eigenvalues E are complex.

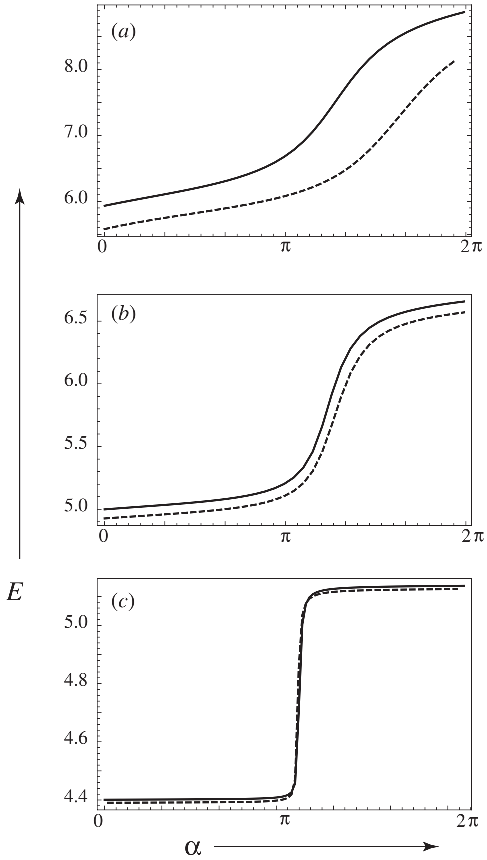

Figure 4. First excited eigenenergy (full curves) and semiclassical approximations (4.18) (dashed curves), for (a) $\eta = 1$, (b) $\eta = 0.5$, (c) $\eta = 0.2$.

For $E > 4$, we can obtain semiclassical approximations to the energies from the formulas (4.17): for the even states, we require $\partial_x \chi(0) = 0$, and for the odd states $\chi(0) = 0$. Thus (cf. (4.18))

$$\cos\frac{A(E)}{2\eta} = \mp\frac{1}{2}\mathrm{i}\exp\left(-2\frac{B(E)}{\eta}\right)\sin\frac{A(E)}{2\eta} \quad \begin{pmatrix}-\text{even}\\ +\text{odd}\end{pmatrix}. \tag{4.20}$$

The small exponential implies that the energies are exponentially close to the real eigenvalues E_{n0} of the hermitian operator for $\alpha = 0$, given by (1.6). Thus elementary expansion gives

$$E_n = E_{n0} + E_{n1}, \tag{4.21}$$

where

$$E_{n1} \approx \pm\mathrm{i}\frac{\eta}{\partial_E A(E_{n0})}\exp\left(-\frac{2B(E_{n0})}{\eta}\right). \tag{4.21}$$

Numerical calculation of some of the resonances for decreasing η indicates that this semiclassical formula is a good approximation.

The fact that equation (2.8) does not generate a hermitian operator when considered on the full x axis motivated the restriction to the half-line $x > 0$. It might appear that this spoils the symmetry between x and p. However, we point out that our whole analysis is essentially unchanged if we start from the momentum, rather than the coordinate, representation, that is exchanging x and p and changing the sign in (2.5); in this sense, the symmetry is preserved.

5. Comparison with Riemann zeta function

To compare the spectrum of the operator representing (1.3) with the set of Riemann zeros, we start by noting that the heights of the zeros are symmetric about $t = 0$, that is, there are zeros at $\pm t_n$. For the operator we have been studying, it follows from the symmetry (3.1) and the 2π periodicity in α that only $\alpha = 0$ and $\alpha = \pi$ give spectra that are symmetric about $E = 0$, so these are the only values we need to consider. We can exclude $\alpha = \pi$ because this gives an eigenvalue at $E = 0$ and there is no Riemann zero with $t = 0$. Therefore we need to compare the Riemann zeros with the eigenvalues for $\alpha = 0$, with asymptotics given by (1.6).

For the Riemann zeros, the mean density of the heights is [1, 4]

$$\begin{aligned} d_{\mathrm{Rsm}}(t) &= \frac{1}{\pi}\partial_t\left(\arg\Gamma\left(\frac{1}{2}+\mathrm{i}t\right) - \frac{t}{2}\log\pi\right) \\ &= \frac{1}{2\pi}\log\frac{t}{2\pi} - \frac{1}{48\pi t^2} + \cdots \end{aligned} \tag{5.1}$$

For our eigenvalues with $\alpha = 0$, (1.4) and (1.6) give the density

$$\begin{aligned} d_{E,\alpha=0}(E) &= \frac{1}{2\pi\eta}\partial_E A(E) = \frac{1}{2\pi\eta}\mathrm{K}\left(1-\frac{16}{E^2}\right) \\ &= \frac{1}{2\pi\eta}\left(\log E + \frac{4}{E^2}(\log E - 1) + \cdots\right). \end{aligned} \tag{5.2}$$

For the leading term to agree with (5.1), we must make the identifications

$$E = \frac{t}{2\pi}, \qquad \eta = \frac{1}{2\pi}, \qquad \text{i.e. } l_x l_p = 2\pi\hbar = h. \tag{5.3}$$

In the variable t, the eigenvalue density is

$$\begin{aligned} d_{t,\alpha=0}(t) &= \frac{1}{2\pi}d_{E,\alpha=0}\left(E = \frac{t}{2\pi}\right) \\ &= \partial_t A\left(\frac{t}{2\pi}\right) = \frac{\mathrm{K}\left(1-\frac{64\pi^2}{t^2}\right)}{2\pi} \\ &= \frac{1}{2\pi}\log\left(\frac{t}{2\pi}\right) + \frac{8\pi}{t^2}\left(\log\left(\frac{t}{2\pi}\right) - 1\right) + \cdots \end{aligned} \tag{5.4}$$

Figure 5 illustrates how the gamma-function formula (5.1) for the Riemann zeros approaches the elliptic-integral formula (5.4) as t increases. For large t, the first correction terms are discrepant and indeed have opposite signs. For the counting functions

$$N(t) = \int_0^t \mathrm{d}t' d(t'), \tag{5.5}$$

the first two terms agree, because the Riemann zero formula is

$$N_{\mathrm{Rsm}}(t) = \frac{t}{2\pi}\left(\log\frac{t}{2\pi} - 1\right) + \frac{7}{8} + \cdots, \tag{5.6}$$

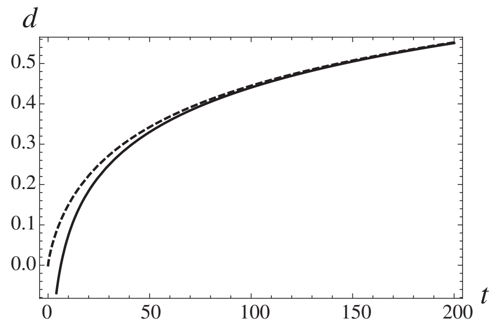

Figure 5. Full curve: exact smoothed density of Riemann zeros (first equality in (5.1)); dashed curve: exact smoothed densityof eigenvalues $E = t/2\pi$ with $\alpha = 0$ (third equality in (5.4)).

while the eigenvalue formula is

$$N_{t,\alpha=0}(t) = \frac{t}{2\pi}\left(\log\left(\frac{t}{2\pi}\right) - 1\right) - \frac{8\pi}{t}\log\left(\frac{t}{2\pi}\right) + \cdots \tag{5.7}$$

6. Concluding remarks

As should be clear from the preceding section, we are not claiming that our hamiltonian (1.3) has an immediate connection with the Riemann zeta function. This is ruled out not only by the fact that the mean eigenvalue density differs from the density of Riemann zeros after the first terms, but by a more fundamental difference in the periodic orbits. For (1.3), there is a single primitive periodic orbit for each energy E; and for the conjectured dynamics underlying the zeta function [4, 8], there is a family of primitive orbits for each 'energy' t, labelled by primes p, with periods $\log p$. This absence of connection with the primes is shared by all variants of xp, and our analysis gives no hint of a resolution of this difficulty.

Our aim is different: to complement existing studies of xp [8, 20] and $x(p + 1/p)$ [10] by displaying a hermitian operator on the whole positive x axis, obtained by unproblematic quantization of a classical hamiltonian symmetric in x and p, that possesses a discrete spectrum reproducing the leading-order density of the Riemann zeros.

Our hamiltonian is interesting in its own right. The square-integrable wavefunctions associated with discrete eigenvalues are solutions of the Schrödinger-like equation (2.8) and (2.9). But the derivation of the boundary condition that guarantees hermiticity requires the integral equation (2.15), whose structure is a consequence of the occurrence of $1/p$ in the classical hamiltonian. The different hermitian operators with the same classical counterpart (1.3)—the different self-adjoint extensions—are parameterised by the angle α. The spiralling of the single eigencurve around the E, α cylinder is reminiscent of the index theorem [21, 22] for the Dirac equation.

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References

[1] Edwards H M 1974 *Riemann's Zeta Function* (New York and London: Academic)
[2] Titchmarsh E C 1986 *The Theory of the Riemann Zeta-Function* (Oxford: Clarendon Press)
[3] Berry M V 1986 Riemann's Zeta function: A model for quantum chaos? *Quantum Chaos and Statistical Nuclear Physics: Proc. 2nd Int. Conf. on Quantum Chaos and 4th Int. Colloquium on Statistical Nuclear Physics (Cuernavaca, México, 6–10 January 1986) (Lecture Notes in Physics* vol 263*)* ed T H Seligman and H Nishioka (Berlin: Springer) pp 1–17
[4] Berry M V and Keating J P 1999 The Riemann zeros and eigenvalue asymptotics *SIAM Rev.* **41** 236–66
[5] Selberg A 1956 Harmonic analysis and discontinuous groups in weakly Riemannian spaces with applications to Dirichlet series *J. Indian Math. Soc.* **20** 47–87
[6] McKean H P 1972 Selberg's trace formula as applied to a compact Riemann surface *Commun. Pure. Appl. Math.* **25** 225–46
[7] Gutzwiller M C 1971 Periodic orbits and classical quantization conditions *J. Math. Phys.* **12** 343–58
[8] Berry M V and Keating J P 1999 $H = xp$ and the Riemann Zeros *Supersymmetry and Trace Formulae: Chaos and Disorder (NATO Science Series B: Physics* vol 370*)* ed I V Lerner, J P Keating and D E Khmelnitskii (New York: Plenum) pp 355–67
[9] Sierra G and Townsend P 2008 Landau levels and Riemann zeros *Phys. Rev. Lett.* **101** 110201
[10] Sierra G and Rodiguez-Laguna J 2011 The $H = xp$ model revisited and the Riemann zeros (arXiv:1102.5356v1 [math-ph])
[11] Wolfram S 1996 *The Mathematica Book* (Cambridge: Cambridge University Press)
[12] DLMF 2010 *NIST Handbook of Mathematical Functions* (Cambridge: Cambridge University Press) http://dlmf.nist.gov
[13] Gustavson K and Abe T 1998 The third boundary condition—was it Robin's? *Math. Intell.* **20** 63–70
[14] Baltes H-P and Hilf E R 1976 *Spectra of Finite Systems* (Mannheim: B-I Wissenschaftsverlag)
[15] Aharonov Y and Bohm D 1959 Significance of electromagnetic potentials in the quantum theory *Phys. Rev.* **115** 485–91
[16] Olariu S and Popescu I I 1985 The quantum effects of electromagnetic fluxes *Rev. Mod. Phys.* **57** 339–436
[17] Dingle R B 1973 *Asymptotic Expansions: Their Derivation and Interpretation* (New York: Academic)
[18] Heading J 1962 *An Introduction to Phase-Integral Methods* (London: Methuen)
[19] Berry M V and Mount K E 1972 Semiclassical approximations in wave mechanics *Rep. Prog. Phys.* **35** 315–97
[20] Srednicki M 2011 The Berry–Keating hamiltonian and the local Riemann hypothesis (arXiv:1104.1850v1 [math-ph])
[21] Shanahan P 1978 *The Atiyah–Singer Index Theorem: An Introduction (Springer Lecture Notes in Mathematics* vol 638*)* ed A Dold and B Eckmann (Berlin: Springer)
[22] Getzler E 1983 Pseudodifferential operators on supermanifolds and the Atiyah-Singer index theorem *Commun. Math. Phys.* **92** 163–78