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# A quantum mechanical model of the Riemann zeros

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**Abstract.** In 1999, Berry and Keating showed that a regularization of the 1D classical Hamiltonian $H = xp$ gives semiclassically the smooth counting function of the Riemann zeros. In this paper, we first generalize this result by considering a phase space delimited by two boundary functions in position and momenta, which induce a fluctuation term in the counting of energy levels. We next quantize the $xp$ Hamiltonian, adding an interaction term that depends on two wavefunctions associated with the classical boundaries in phase space. The general model is solved exactly, obtaining a continuum spectrum with discrete bound states embedded in it. We find the boundary wavefunctions associated with the Berry–Keating regularization, for which the average Riemann zeros become resonances. A spectral realization of the Riemann zeros is achieved exploiting the symmetry of the model under the exchange of position and momenta which is related to the duality symmetry of the zeta function. The boundary wavefunctions, giving rise to the Riemann zeros, are found using the Riemann–Siegel formula of the zeta function. Other Dirichlet L-functions are shown to find a natural realization in the model.

## Contents



## 1. Introduction

At the beginning of the 20th century Polya and Hilbert made the bold conjecture that the imaginary part of the Riemann zeros could be the oscillation frequencies of a physical system. If true this suggestion would imply a proof of the celebrated Riemann hypothesis (RH). The importance of this conjecture lies in its connection with prime numbers. If the RH is true then the statistical distribution of the primes will be constrained in the most favourable way [1, 2]. Otherwise, in the words of Bombieri, the failure of the RH would create havoc in the distribution of the prime numbers [3] (see also [4]–[7][1] for reviews on the RH).

After the advent of quantum mechanics, the Polya–Hilbert conjecture was formulated as the existence of a self-adjoint operator whose spectrum contains the imaginary part of the Riemann zeros. This conjecture was for a long time regarded as a wild speculation until the works of Selberg in the 50s and those of Montgomery in the 70s. Selberg found a remarkable duality between the length of geodesics on a Riemann surface and the eigenvalues of the Laplacian operator defined on it [8]. This duality is encapsulated in the so called Selberg trace formula, which has a strong similarity to the Riemann explicit formula relating the zeros and the prime numbers. The Riemann zeros would correspond to the eigenvalues, and the primes to the geodesics. This classical versus quantum version of the primes and the zeros is also at the heart of the so-called quantum chaos approach to the RH.

Quite independently of Selberg's work, Montgomery showed that the Riemann zeros are distributed randomly and obey locally the statistical law of the random matrix theory (RMT) [9]. The RMT was originally proposed to explain the chaotic behaviour of the spectra of nuclei but it has applications in other branches of physics, especially in condensed matter [10]. There are several universality classes of random matrices, and it turns out that the one related to the Riemann zeros is the Gaussian unitary ensemble (GUE) associated with random hermitean

[1] See Watkins M at http://secamlocal.ex.ac.uk/∼mwatkins/zeta/physics.htm for a comprehensive review on several approaches to the RH.

matrices. Montgomery's analytical results found an impressive numerical confirmation in the works of Odlyzko in the 80s, so that the GUE law, as applied to the Riemann zeros is nowadays called the Montgomery–Odlyzko law [11]. An important hint suggested by this law is that the Polya–Hilbert Hamiltonian $H$ must break the time reversal symmetry. The reason for this is that the GUE statistics describes random Hamiltonians where this symmetry is broken. A simple example is provided by materials with impurities subject to an external magnetic field, as in the quantum Hall effect.

A further step in the Polya–Hilbert–Montgomery–Odlyzko pathway was taken by Berry [12, 13], who noticed a similarity between the formula yielding the fluctuations of the number of zeros, around its average position $E_n \sim 2\pi n/\log n$, and a formula giving the fluctuations of the energy levels of a Hamiltonian obtained by the quantization of a classical chaotic system [14]. The comparison between these two formulae suggests that the prime numbers $p$ correspond to the isolated periodic orbits whose period is $\log p$. In the quantum chaos scenario the prime numbers appear as classical objects, while the Riemann zeros are quantal. This classical/quantum interpretation of the primes/zeros is certainly reminiscent of the one underlying the Selberg trace formula mentioned earlier. A success of the quantum chaos approach is that it explains the deviations from the GUE law of the zeros found numerically by Odlyzko. The similarity between the fluctuation formulae described above, while rather appealing, has a serious drawback observed by Connes which has to do with an overall sign difference between them [15]. It is as if the periodic orbits were missing in the underlying classical chaotic dynamics, a fact that is difficult to understand physically. This and other observations led Connes to propose an abstract approach to the RH based on discrete mathematical objects known as adeles [15]. The final outcome of Connes' work is a trace formula whose proof, not yet found, amounts to that of a generalized version of the RH. In Connes' approach there is an operator, which plays the role of the Hamiltonian, whose spectrum is a continuum with missing spectral lines corresponding to the Riemann zeros. We are thus confronted with two possible physical realizations of the Riemann zeros, either as point-like spectra or as missing spectra in a continuum. Later on we shall see that both pictures can be reconciled in a QM model having a discrete spectra embedded in a continuum.

The next step within the Polya–Hilbert framework came in 1999 when Berry and Keating [16, 17] on one hand and Connes [15] on the other, proposed that the classical Hamiltonian $H = xp$, where $x$ and $p$ are the position and momenta of a one-dimensional (1D) particle, is closely related to the Riemann zeros. This striking suggestion was based on a semiclassical analysis of $H = xp$, which led these authors to reach quite opposite conclusions regarding the possible spectral interpretation of the Riemann zeros. The origin of the disagreement is due to the choice of different regularizations of $H = xp$. Berry and Keating chose a Planck cell regularization in which case the smooth part of the Riemann zeros appears semiclassically as discrete energy levels. Connes, on the other hand chose an upper cutoff for the position and momenta which gives semiclassically a continuum spectrum where the smooth zeros are missing. All these semiclassical results are heuristic and so far lack a consistent quantum version. It is the aim of this paper to provide such a quantum version in the hope that it will shed new light concerning the spectral realization of the Riemann zeros.

The organization of the paper is as follows. In section 2, we review the semiclassical approaches to $H = xp$ due to Berry, Keating and Connes who gave an heuristic derivation of the asymptotic behaviour of the smooth part of the Riemann zeros. In section 3, we generalize the semiclassical Berry–Keating (BK) Planck cell regularization of $xp$ by means of two classical functions which define a *wiggly* boundary for the allowed semiclassical region in phase space. This generalization allows us to explain semiclassically the fluctuation term in the spectrum. In section 4, we define the quantum Hamiltonian associated with the semiclassical approach introduced above. The Hamiltonian is given by the quantization of $H = xp$ plus an interaction term that depends on two generic boundary wavefunctions and we solve the associated Schrödinger equation finding the exact eigenfunctions and eigenenergies in terms of a function $\mathcal{F}(E)$ which plays the role of a Jost function for this model, and whose analyticity properties are studied in section 5. In section 6, we find the boundary wavefunctions that give rise to the quantum version of the semiclassical BK model for the smooth zeros of the Riemann zeta function, which are common to all the even Dirichlet L-functions. We also find the boundary wavefunctions associated with the smooth approximation of the zeros of the odd Dirichlet L-functions. In section 7, we quantize the relation between the fluctuation part of the spectrum and the semiclassical phase boundaries, obtaining the equations satisfied by the boundary wavefunctions, and we solve them explicitly. Finally, using the duality properties of these wavefunctions and the Riemann–Siegel formula of the zeta function we find a model whose Jost function is proportional to the zeta function. From this fact, and making some additional assumptions, we show that the Riemann zeros on the critical line are bound states of the model. However, we cannot exclude the existence of zeros outside the critical line, which would imply a proof of the RH. We describe in an appendix the computation of the wavefunctions associated with the smooth and exact Riemann zeros.

The present work is closely related to those in [18]–[20], where we studied an interacting version of the $xp$ Hamiltonian based on the relation of this model with the so called Russian doll model of superconductivity [21]–[23]. For a field theoretical approach to the RH inspired by the latter works, see [24]. We would also like to mention some important differences between the present paper and those of [18]–[20]. First of all, the position variable $x$ was chosen in [18]–[20] to belong to the finite interval $(1, N)$ with $N \to \infty$, while in this paper we choose the half line $(0, \infty)$ which gives a more symmetric treatment between the position and momentum variables. Secondly, in the earlier references the interaction term was added to the inverse Hamiltonian $1/(xp)$, while in this paper we add the interaction directly to the Hamiltonian $xp$, which is more natural from a physical viewpoint. We have also tried to make an extensive use of the duality symmetry of the Riemann zeta function reflected in the functional relation it satisfies.

## 2. Semiclassical approach

The classical Berry–Keating–Connes (BKC) Hamiltonian [15]–[17]

$$H_0^{\mathrm{cl}} = xp \tag{2.1}$$

has classical trajectories given by the hyperbolas (see figure 1(a))

$$x(t) = x_0 \mathrm{e}^{t}, \qquad p(t) = p_0 \mathrm{e}^{-t}. \tag{2.2}$$

The dynamics is unbounded, so one should not expect a discrete spectrum even at the semiclassical level. To overcome this difficulty, Berry and Keating proposed in 1999 to restrict the phase space of the $xp$ model to those points $(x, p)$ where $|x| > l_x$ and $|p| > l_p$, with

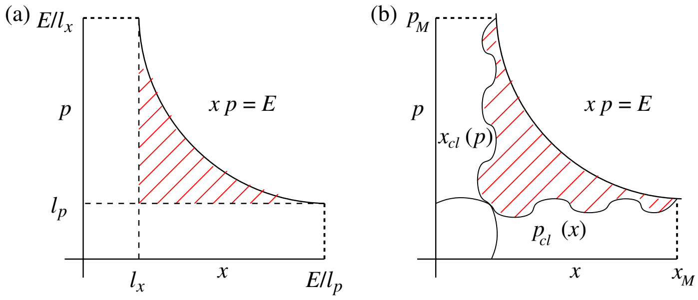


**Figure 1.** (a) A classical trajectory (2.2). The region in shadow is the allowed phase space of the semiclassical regularizations of Berry and Keating. (b) Generalization of the phase space region given by equations (3.1).

$l_x\, l_p = 2\pi\hbar$. These constraints lead to a finite number of semiclassical states, $\mathcal{N}(E)$, with energy between 0 and $E$ given by

$$\mathcal{N}(E) = \frac{A}{2\pi\hbar}, \tag{2.3}$$

where $A$ is the area of the allowed phase space region below the curve $E = xp$. The result, in units $\hbar = 1$ is

$$\mathcal{N}_{\rm BK}(E) = \frac{E}{2\pi}\left(\log\frac{E}{2\pi} - 1\right) + 1, \tag{2.4}$$

which agrees with the asymptotic limit of the smooth part of the formula giving the number of Riemann zeros whose imaginary part lies in the interval $(0, E)$,

$$\langle\mathcal{N}(E)\rangle \sim \frac{E}{2\pi}\left(\log\frac{E}{2\pi} - 1\right) + \frac{7}{8} + O(E^{-1}). \tag{2.5}$$

The exact formula for the number of zeros, $\mathcal{N}_{\rm R}(E)$, due to Riemann, also contains a fluctuation term which depends on the zeta function [1] (see figure 2),

$$\begin{aligned} \mathcal{N}_{\rm R}(E) &= \langle\mathcal{N}(E)\rangle + \mathcal{N}_{\rm fl}(E), \\ \langle\mathcal{N}(E)\rangle &= \frac{\theta(E)}{\pi} + 1, \\ \mathcal{N}_{\rm fl}(E) &= \frac{1}{\pi}{\rm Im}\log\zeta\left(\frac{1}{2} + {\rm i}E\right), \end{aligned} \tag{2.6}$$

where $\theta(E)$ is the phase of the Riemann zeta function $\zeta(1/2 - {\rm i}E)$,

$$\theta(E) = {\rm Im}\log\Gamma\left(\frac{1}{4} + \frac{\rm i}{2}E\right) - \frac{E}{2}\log\pi, \tag{2.7}$$

whose asymptotic expansion

$$\theta(E) = \frac{E}{2}\log\left(\frac{E}{2\pi}\right) - \frac{E}{2} - \frac{\pi}{8} + O(E^{-1}) \tag{2.8}$$

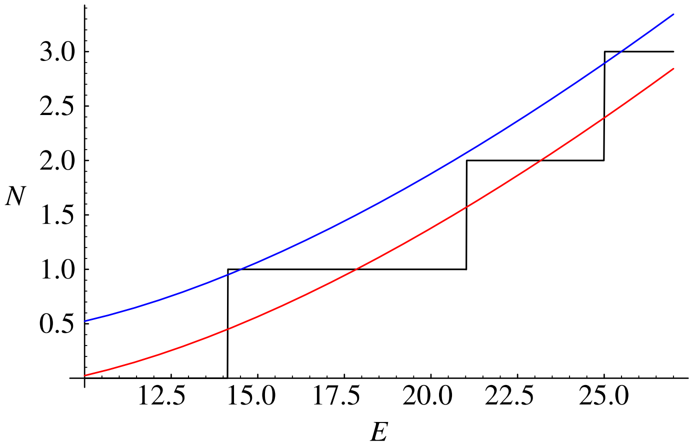


**Figure 2.** Number of Riemann zeros in the interval $(0, E)$: black: exact formula (2.6), red: smooth function $\langle \mathcal{N}(E) \rangle$ and blue: $\langle \mathcal{N}(E) \rangle + 1/2$.

yields (2.5). The function $\zeta(s)$, for $\mathrm{Re}\, s > 1$, can be related to the prime numbers $p$ thanks to the Euler product formula

$$\zeta(s) = \prod_{p>1} \frac{1}{1 - p^{-s}}, \qquad \mathrm{Re}\, s > 1. \tag{2.9}$$

This expression diverges if $\mathrm{Re}\, s = 1/2$, however one can heuristically use it to write the fluctuation term in (2.6) as

$$\mathcal{N}_{\mathrm{fl}}(E) = -\frac{1}{\pi} \sum_p \sum_{m=1}^{\infty} \frac{1}{m p^{m/2}} \sin(mE \log p), \tag{2.10}$$

which gives a reasonable result after truncating the sum over the primes. As observed by Berry, equation (2.10) resembles formally the fluctuation part of the spectrum of a classical 1D chaotic Hamiltonian with isolated periodic orbits

$$\mathcal{N}_{\mathrm{fl}}(E) = \frac{1}{\pi} \sum_{\gamma_{\mathrm{p}}} \sum_{m=1}^{\infty} \frac{1}{m 2\sinh(m\lambda_{\mathrm{p}}/2)} \sin(S_{\mathrm{cl}}(E)), \tag{2.11}$$

where $\gamma_{\mathrm{p}}$ denotes the primitive periodic orbits, the label $m$ describes the windings of those orbits, $\pm\lambda_{\mathrm{p}}$ are the instability exponents and $S_{\mathrm{cl}}(E)$ is the classical action, which is equal to $mET_{\gamma_{\mathrm{p}}}$, with $T_{\gamma_{\mathrm{p}}}$ the period of $\gamma_{\mathrm{p}}$. Comparing (2.10) and (2.11), Berry conjectured the existence of a classical chaotic Hamiltonian whose primitive periodic orbits would be labelled by the prime numbers $p = 2, 3, \ldots$, with periods $T_{\mathrm{p}} = \log p$ and instability exponents $\lambda_{\mathrm{p}} = \pm \log p$ [12, 13]. Moreover, since each orbit is counted once, the Hamiltonian must break time reversal (otherwise there would be a factor $2/\pi$ in front of equation (2.10) instead of $1/\pi$). The quantization of this classical chaotic Hamiltonian would likely contain the Riemann zeros in its spectrum. This idea is the key of the quantum chaos approach to the RH.

Besides the fact that the earlier Hamiltonian has not yet been found there is the Connes criticism that the similarity between equations (2.10) and (2.11) fails in two issues. The first is the overall minus sign in (2.10) as compared to (2.11), and the second is that the term $2\sinh(m\lambda_{\mathrm{p}}/2)$ only becomes $p^{m/2}$ when $m \to \infty$. Connes relates the *minus sign* problem to an alternative interpretation of the Riemann zeros as missing spectral lines as opposed to the conventional one. This interpretation is based on a different regularization scheme for the $xp$ Hamiltonian. In [15], Connes restricts the phase space of the model to be $|x| < \Lambda$, $|p| < \Lambda$, where $\Lambda$ is a cutoff which is sent to infinite at the end of the calculation. The number of semiclassical states is given now by

$$\mathcal{N}_{\rm C}(E) = \frac{E}{\pi}\log\Lambda - \frac{E}{2\pi}\left(\log\frac{E}{2\pi} - 1\right), \qquad (2.12)$$

where the first term leads, in the limit $\Lambda \to \infty$, to a continuum while the second term coincides with minus the average position of the Riemann zeros (2.4). A possible interpretation of these results is that the Riemann zeros are missing spectral lines in a continuum, which is in apparent contradiction with the BK interpretation of the zeros as bound states. As we shall show below both interpretations can be reconciled at the quantum level where the Riemann zeros appear as discrete spectra embbeded in a continuum of states.

## 3. Semiclassical treatment of the fluctuations

The quantum chaos approach suggests that the fluctuation part of the spectrum of the yet unknown Riemann Hamiltonian has a classical origin related to the prime numbers. Taking into account the BK heuristic derivation of the smooth part of the spectrum, it is tempting to extend the semiclassical approach in order to explain the fluctuation term in the Riemann formula for the zeros. The simplest idea is to generalize the allowed phase space of the $xp$ Hamiltonian replacing the boundaries $|x| = l_x$ and $|p| = l_p$ by two curves $x_{\rm cl}(p)$ and $p_{\rm cl}(x)$, such that (see figure 1(b))

$$x > x_{\rm cl}(p), \qquad |p| > p_{\rm cl}(x), \qquad (3.1)$$

where $x_{\rm cl}(p)$ and $p_{\rm cl}(x)$, are positive functions satisfying

$$\begin{aligned} &x_{\rm cl}(p) = x_{\rm cl}(-p) > 0, \quad \forall p \in \mathbb{R}, \\ &p_{\rm cl}(x) > 0, \qquad\qquad\quad \forall x \in \mathbb{R}_+. \end{aligned} \qquad (3.2)$$

These conditions split the allowed phase space into two disconnected regions in the first and forth quadrants of the $xp$ plane. Notice that $x$ is always positive while $p$ can be either positive or negative. The BK boundaries obviously correspond to the choice

$$\text{BK}: x_{\rm cl}(p) = l_x, \qquad p_{\rm cl}(x) = l_p. \qquad (3.3)$$

For the extended boundary conditions (BCs) the minimal distance $l_x$ and minimal momentum $l_p$ can be defined as the intersection point of the curves, $x_{\rm cl}(p)$ and $p_{\rm cl}(x)$, which we shall assume to be unique and to satisfy

$$x_{\rm cl}(l_p) = l_x, \qquad p_{\rm cl}(l_x) = l_p. \qquad (3.4)$$

The classical $xp$ Hamiltonian together with the BK conditions have the exchange symmetry

$$\frac{x}{l_x} \leftrightarrow \frac{p}{l_p}, \qquad (3.5)$$

whose generalization to the extended model is

$$\frac{x_{\rm cl}(l_p x/l_x)}{l_x} = \frac{p_{\rm cl}(x)}{l_p}. \qquad (3.6)$$

The counting of semiclassical states is based again on equation (2.3). The area below the curve $E = xp$ and bounded by the conditions (3.1) is given by (see figure 1(b))

$$A = \int_{l_x}^{x_I} \mathrm{d}x \int_{p_{\mathrm{cl}}(x)}^{l_p x/l_x} \mathrm{d}p + \int_{x_I}^{x_M} \mathrm{d}x \int_{p_{\mathrm{cl}}(x)}^{E/x} \mathrm{d}p + \int_{l_p}^{p_I} \mathrm{d}p \int_{x_{\mathrm{cl}}(p)}^{l_x p/l_p} \mathrm{d}x + \int_{p_I}^{p_M} \mathrm{d}p \int_{x_{\mathrm{cl}}(p)}^{E/p} \mathrm{d}x. \tag{3.7}$$

The quantities $x_M$, $p_M$ (resp. $x_I$, $p_I$) are the position and momenta of the points where the curve $E = xp$ intersects the boundaries $p_{\mathrm{cl}}(x)$, $x_{\mathrm{cl}}(p)$ (resp. the line $x/l_x = p/l_p$), and satisfy,

$$E = x_M\, p_{\mathrm{cl}}(x_M) = x_{\mathrm{cl}}(p_M)\, p_M = x_I\, p_I, \qquad \frac{x_I}{l_x} = \frac{p_I}{l_p}. \tag{3.8}$$

Integration of (3.7) yields

$$A = E \log\left(\frac{E}{l_x l_p}\right) + E - l_x l_p - E \log\left(\frac{p_{\mathrm{cl}}(x_M)}{l_p}\right) - E \log\left(\frac{x_{\mathrm{cl}}(p_M)}{l_x}\right) - \int_{l_x}^{x_M} \mathrm{d}x\, p_{\mathrm{cl}}(x) - \int_{l_p}^{p_M} \mathrm{d}p\, x_{\mathrm{cl}}(p). \tag{3.9}$$

Partially integrating the last two terms in (3.9) and dividing by $h = l_x l_p = 2\pi (\hbar = 1)$, the semiclassical value of $\mathcal{N}(E)$ reads

$$\mathcal{N}(E) = \mathcal{N}_{\mathrm{BK}}(E) - \frac{E}{2\pi} \log\left(\frac{p_{\mathrm{cl}}(x_M)}{l_p}\right) - \frac{E}{2\pi} \log\left(\frac{x_{\mathrm{cl}}(p_M)}{l_x}\right) + \int_{l_x}^{x_M} \frac{\mathrm{d}x}{2\pi} x \frac{\mathrm{d}p_{\mathrm{cl}}(x)}{\mathrm{d}x} + \int_{l_p}^{p_M} \frac{\mathrm{d}p}{2\pi} p \frac{\mathrm{d}x_{\mathrm{cl}}(p)}{\mathrm{d}p}. \tag{3.10}$$

The BK conditions (3.3) of course reproduce equation (2.4). More general boundary functions induce a fluctuation term in the counting formula of a form which recalls equation (2.6). Let us denote this term as

$$n_{\mathrm{fl}}(E) = -\frac{E}{2\pi} \log\left(\frac{p_{\mathrm{cl}}(x_M)}{l_p}\right) - \frac{E}{2\pi} \log\left(\frac{x_{\mathrm{cl}}(p_M)}{l_x}\right) + \int_{l_x}^{x_M} \frac{\mathrm{d}x}{2\pi} x \frac{\mathrm{d}p_{\mathrm{cl}}(x)}{\mathrm{d}x} + \int_{l_p}^{p_M} \frac{\mathrm{d}p}{2\pi} p \frac{\mathrm{d}x_{\mathrm{cl}}(p)}{\mathrm{d}p} \tag{3.11}$$

so that

$$\mathcal{N}(E) = \mathcal{N}_{\mathrm{BK}}(E) + n_{\mathrm{fl}}(E). \tag{3.12}$$

Taking the derivative of (3.11) with respect to $E$, and using equations (3.8) one gets

$$\frac{\mathrm{d}n_{\mathrm{fl}}(E)}{\mathrm{d}E} = -\frac{1}{2\pi} \log\left(\frac{p_{\mathrm{cl}}(x_M)}{l_p}\right) - \frac{1}{2\pi} \log\left(\frac{x_{\mathrm{cl}}(p_M)}{l_x}\right), \tag{3.13}$$

which implies that the boundary functions are related to the fluctuation part of the density of states. A further simplification is achieved imposing the $xp$ symmetry (3.6)

$$\frac{p_{\mathrm{cl}}(x_M)}{l_p} = \frac{x_{\mathrm{cl}}(p_M)}{l_x}, \qquad \frac{p_M}{l_p} = \frac{x_M}{l_x}, \tag{3.14}$$

which leads to

$$\frac{\mathrm{d}n_{\mathrm{fl}}(E)}{\mathrm{d}E} = -\frac{1}{\pi} \log\left(\frac{p_{\mathrm{cl}}(x_M)}{l_p}\right) = -\frac{1}{\pi} \log\left(\frac{x_{\mathrm{cl}}(p_M)}{l_x}\right). \tag{3.15}$$

Hence, $xp$-symmetric boundary functions $p_{\rm cl}(x_M)$ and $x_{\rm cl}(p_M)$ are completely fixed by the density of the fluctuations. To find $p_{\rm cl}(x)$, one combines (3.15) and (3.8)

$$p_{\rm cl}(x_M) = l_p\, {\rm e}^{-\pi n'_{\rm fl}(E)} = \frac{E}{x_M}, \qquad n'_{\rm fl}(E) = \frac{{\rm d}n_{\rm fl}(E)}{{\rm d}E}, \tag{3.16}$$

which gives $x_M$ as a function of $E$

$$x_M = \frac{E}{l_p}\, {\rm e}^{\pi n'_{\rm fl}(E)}. \tag{3.17}$$

If $n_{\rm fl}(E) = 0$, the latter equations reproduce the BK boundary conditions (3.4). Equation (3.17) gives $x_M$ as a function of $E$ and it is monotonically increasing, provided

$$\frac{{\rm d}x_M(E)}{{\rm d}E} > 0 \quad \Longrightarrow \quad 1 + \pi E \frac{{\rm d}^2 n_{\rm fl}(E)}{{\rm d}E^2} > 0. \tag{3.18}$$

Under this condition, we can express $E$ as a function of $x_M$ and replace it in (3.16), obtaining the boundary function $p_{x_M} = E(x_M)/x_M$. In this case, the inverse problem of finding a Hamiltonian given the spectrum has a unique solution at the semiclassical level. If the fluctuations are strong enough at some energies, then condition (3.18) could be violated implying that $E = E(x)$ as well as $p_{\rm cl}(x)$ will be multivalued functions. This gives rise to a manifold of boundary functions, each one having discontinuities at some values of $x$.

## 4. The quantum model

In this section, we shall give a quantum version of the semiclassical results obtained above. The starting point is the quantization of the classical hamiltonian $H_0^{\rm cl} = xp$. Let us consider the usual normal ordered expression

$$H_0 = \tfrac{1}{2}(xp + px) = -{\rm i}\left(x\tfrac{\rm d}{{\rm d}x} + \tfrac{1}{2}\right), \tag{4.1}$$

where $p = -{\rm i}\,{\rm d}/{\rm d}x$. In [19, 25] it was shown that $H_0$ becomes a self-adjoint operator in two cases where the domain of the $x$ variable are chosen as: (1) $0 < x < \infty$ or (2) $a < x < b$ with $a$ and $b$ finite. For the purpose of this paper, we shall keep to case 1. Case 2 was discussed at length in [19]. Since $x > 0$ one can write (4.1) as

$$H_0 = x^{1/2} p x^{1/2}, \qquad x > 0. \tag{4.2}$$

The exact eigenfunctions of (4.2) are given by

$$\phi_E(x) = \frac{1}{\sqrt{2\pi}} \frac{1}{x^{1/2-{\rm i}E}}, \qquad E \in \mathbb{R}, \tag{4.3}$$

where the eigenenergies $E$ belong to the real line. The normalization of (4.3) is the appropiate one for a continuum spectra,

$$\langle \phi_E | \phi_{E'} \rangle = \int_0^\infty {\rm d}x\, \phi_E^*(x) \phi_{E'}(x) = \delta(E - E'). \tag{4.4}$$

The quantum Hamiltonian associated to the semiclassical approach is

$$H = H_0 + {\rm i}(|\psi_a\rangle\langle\psi_b| - |\psi_b\rangle\langle\psi_a|), \tag{4.5}$$

where $\psi_a$ and $\psi_b$ are two wavefunctions which we take to be real for the Hamiltonian to be hermitean and with eigenvalues appearing in pairs $E, -E$. In this section, we shall give the general solution of the Schrödinger equation associated to the Hamiltonian (4.5), for generic choices of $\psi_{a,b}(x)$. Later on, in section 7, we shall relate $\psi_{a,b}(x)$ to the boundary functions $p_{\rm cl}(x)$ and $x_{\rm cl}(p)$, of the semiclassical model, proving under certain assumptions that the energy spectrum of the quantum model agrees with the semiclassical results derived in the previous section. This justifies *a posteriori* the choice of the Hamiltonian (4.5).

The Schrödinger equation for an eigenstate $\psi_E(x)$ with energy $E$ of the Hamiltonian (4.5) is given by the integro–differential equation

$$-{\rm i}\left(x\frac{{\rm d}}{{\rm d}x}+\frac{1}{2}\right)\psi_E(x)+{\rm i}\psi_a(x)\int_0^\infty {\rm d}y\;\psi_b(y)\psi_E(y)-{\rm i}\psi_b(x)\int_0^\infty {\rm d}y\;\psi_a(y)\psi_E(y) = E\psi_E(x). \tag{4.6}$$

Let us introduce the variable $q$

$$q=\log x,\qquad q\in\mathbb{R} \tag{4.7}$$

and the overlap integrals

$$\begin{aligned} A &= \langle\psi_a|\psi_E\rangle = \int_0^\infty {\rm d}x\;\psi_a(x)\psi_E(x),\\ B &= \langle\psi_b|\psi_E\rangle = \int_0^\infty {\rm d}x\;\psi_b(x)\psi_E(x), \end{aligned} \tag{4.8}$$

which depend on $E$. Using these definitions equation (4.6) becomes

$$-{\rm i}\left(\frac{{\rm d}}{{\rm d}q}+\frac{1}{2}\right)\psi_E(q)+{\rm i}(B\psi_a(q)-A\psi_b(q))=E\psi_E(q). \tag{4.9}$$

The general solution of this equation is given by

$$\psi_E(q)={\rm e}^{-(1/2-{\rm i}E)q}\left[C_0+\int_{-\infty}^q {\rm d}q'\;{\rm e}^{(1/2-{\rm i}E)q'}(B\psi_a(q')-A\psi_b(q'))\right], \tag{4.10}$$

where $C_0$ is an integration constant. It is convenient to define the functions

$$\begin{aligned} a(q)&={\rm e}^{q/2}\psi_a(q), &\qquad \psi_a(x)&=\frac{a(x)}{\sqrt{x}},\\ b(q)&={\rm e}^{q/2}\psi_b(q), &\qquad \psi_b(x)&=\frac{b(x)}{\sqrt{x}} \end{aligned} \tag{4.11}$$

so that

$$\psi_E(q)={\rm e}^{-(1/2-{\rm i}E)q}\left[C_0+\int_{-\infty}^q {\rm d}q'{\rm e}^{-{\rm i}Eq'}(Ba(q')-Ab(q'))\right]. \tag{4.12}$$

An alternative way to express (4.12) is

$$\psi_E(q)={\rm e}^{-(1/2-{\rm i}E)q}\left[C_\infty-\int_q^\infty {\rm d}q'{\rm e}^{-{\rm i}Eq'}(Ba(q')-Ab(q'))\right], \tag{4.13}$$

where $C_\infty$ is related to $C_0$ by

$$C_\infty=C_0+B\hat{a}(-E)-A\hat{b}(-E), \tag{4.14}$$

where

$$\hat{f}(E) = \int_{-\infty}^{\infty} \mathrm{d}q\, \mathrm{e}^{\mathrm{i}Eq} f(q), \qquad f = a, b. \tag{4.15}$$

We shall assume that $a(q)$ and $b(q)$ satisfy

$$\begin{aligned} &\lim_{q\to-\infty} \int_{-\infty}^{q} \mathrm{d}q'\, \mathrm{e}^{-\mathrm{i}Eq'} f(q') = 0, \qquad f = a, b, \\ &\lim_{q\to\infty} \int_{q}^{\infty} \mathrm{d}q'\, \mathrm{e}^{-\mathrm{i}Eq'} f(q') = 0, \qquad f = a, b, \end{aligned} \tag{4.16}$$

which implies that the asymptotic behaviour of $\psi_E(x)$ is dominated by $C_0$ and $C_\infty$, i.e.

$$\lim_{x\to 0} \psi_E(x) = \frac{C_0}{x^{1/2-\mathrm{i}E}}, \qquad \lim_{x\to\infty} \psi_E(x) = \frac{C_\infty}{x^{1/2-\mathrm{i}E}}. \tag{4.17}$$

Plugging (4.12) into (4.8) yields the relation between the constants $A$, $B$ and $C_0$,

$$\begin{pmatrix} 1+S_{a,b} & -S_{a,a} \\ S_{b,b} & 1-S_{b,a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = C_0 \begin{pmatrix} \hat{a}(E) \\ \hat{b}(E) \end{pmatrix}, \tag{4.18}$$

where the functions $S_{f,g}(E)$ with $f, g = a, b$ are defined by[2]

$$S_{f,g}(E) = \int_{-\infty}^{\infty} \mathrm{d}q\, \mathrm{e}^{\mathrm{i}Eq}\, f(q) \int_{-\infty}^{q} \mathrm{d}q'\, \mathrm{e}^{-\mathrm{i}Eq'}\, g(q'). \tag{4.19}$$

Similarly, introducing (4.13) into (4.8) yields

$$\begin{pmatrix} 1-\tilde{S}_{a,b} & \tilde{S}_{a,a} \\ -\tilde{S}_{b,b} & 1+\tilde{S}_{b,a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = C_\infty \begin{pmatrix} \hat{a}(E) \\ \hat{b}(E) \end{pmatrix}, \tag{4.20}$$

where

$$\tilde{S}_{f,g}(E) = \int_{-\infty}^{\infty} \mathrm{d}q\, \mathrm{e}^{\mathrm{i}Eq}\, f(q) \int_{q}^{\infty} \mathrm{d}q'\, \mathrm{e}^{-\mathrm{i}Eq'}\, g(q'). \tag{4.21}$$

This function is related to $S_{f,g}$ in two ways,

$$\tilde{S}_{f,g}(E) = -S_{f,g}(E) + \hat{f}(E)\, \hat{g}(-E), \tag{4.22}$$

$$\tilde{S}_{f,g}(E) = S_{g,f}(-E). \tag{4.23}$$

To derive these equations one makes a change of order in the integration. Combining (4.22) and (4.23) one obtains the *shuffle* relation

$$S_{f,g}(E) + S_{g,f}(-E) = \hat{f}(E)\, \hat{g}(-E). \tag{4.24}$$

The terminology is borrowed from the theory of multiple zeta functions where there is a similar relation between the two variable Euler–Zagier zeta function $\zeta(s_1, s_2)$, and the Riemann zeta function $\zeta(s)$ [26, 27].

The solutions of the equations (4.18) and (4.20) depend on the determinant of the associated $2 \times 2$ matrices given by

$$\begin{aligned} \mathcal{F}(E) &= 1 + S_{a,b} - S_{b,a} + S_{a,a}S_{b,b} - S_{a,b}S_{b,a}, \\ \tilde{\mathcal{F}}(E) &= 1 - \tilde{S}_{a,b} + \tilde{S}_{b,a} + \tilde{S}_{a,a}\tilde{S}_{b,b} - \tilde{S}_{a,b}\tilde{S}_{b,a}, \end{aligned} \tag{4.25}$$

[2] The $S_{f,g}(z)$ differs in a sign respect to the one considered [19, 20].

which are related by (4.23)

$$\tilde{\mathcal{F}}(E) = \mathcal{F}(-E). \tag{4.26}$$

Moreover, since $a(x)$ and $b(x)$ are real functions one has

$$S^*_{f,g}(E) = S_{f,g}(-E^*), \tag{4.27}$$

which in turn implies

$$\mathcal{F}^*(E) = \mathcal{F}(-E^*). \tag{4.28}$$

After these observations, we can return to the solution of (4.18) and (4.20). We shall distinguish two cases: (1) $\mathcal{F}(E) \neq 0$ and (2) $\mathcal{F}(E) = 0$, where $E$ is real since it is an eigenvalue of the Hamiltonian (4.5).

**Case 1:** $\mathcal{F}(E) \neq 0$
Equation (4.28) implies that $\mathcal{F}(-E) \neq 0$ and therefore $A$ and $B$ can be expressed in two different ways,

$$A = \frac{C_0}{\mathcal{F}(E)}\big[(1 - S_{b,a})\,\hat{a}(E) + S_{a,a}\,\hat{b}(E)\big] = \frac{C_\infty}{\mathcal{F}(-E)}\big[(1 + \tilde{S}_{b,a})\,\hat{a}(E) - \tilde{S}_{a,a}\,\hat{b}(E)\big], \tag{4.29}$$

$$B = \frac{C_0}{\mathcal{F}(E)}\big[-S_{b,b}\,\hat{a}(E) + (1 + S_{a,b})\,\hat{b}(E)\big] = \frac{C_\infty}{\mathcal{F}(-E)}\big[\tilde{S}_{b,b}\,\hat{a}(E) + (1 - \tilde{S}_{a,b})\,\hat{b}(E)\big]. \tag{4.30}$$

Now using equation (4.22), these equations reduce to

$$\frac{C_0}{C_\infty} = \frac{\mathcal{F}(E)}{\mathcal{F}(-E)}, \tag{4.31}$$

which by equation (4.28) is a pure phase for $E$ real. Hence, up to an overall factor, the integration constants for this solution can be chosen as

$$\begin{aligned} C_0 &= \mathcal{F}(E), \\ C_\infty &= \mathcal{F}(-E), \\ A &= (1 - S_{b,a})\,\hat{a}(E) + S_{a,a}\,\hat{b}(E), \\ B &= -S_{b,b}\,\hat{a}(E) + (1 + S_{a,b})\,\hat{b}(E). \end{aligned} \tag{4.32}$$

Since the constants $C_0$ and $C_\infty$ do not vanish, the wavefunction is non normalizable near the origin and infinity (recall equation (4.17)) and therefore they correspond to scattering states. Of course they will be normalizable in the distributional sense.

**Case 2:** $\mathcal{F}(E) = 0$
The integration constants can be chosen as

$$\begin{aligned} C_0 &= 0, \\ C_\infty &= 0, \\ A &= S_{a,a}, \\ B &= (1 + S_{a,b}), \end{aligned} \tag{4.33}$$

which solves equations (4.18) and (4.20). Since $C_0 = C_\infty = 0$, the leading term of the behaviour of $\psi_E(x)$ vanish near the origin and infinity and under appropiate conditions on $\psi_{a,b}$, the state

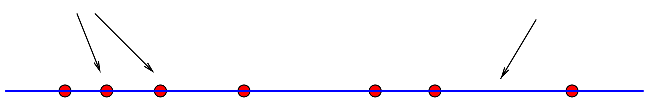


**Figure 3.** Pictorial representation of the spectrum of the model. The bound states are the points where $\mathcal{F}(E) = 0$, which are embedded in a continuum of scattering states.

$\psi_E$ will be normalizable corresponding to a bound state. In the appendix, we compute the norm of these states.

Hence, the generic spectrum of the Hamiltonian (4.5) consists of a continuum covering the whole real line with, eventually, some isolated bound states embedded in it, whenever $\mathcal{F}(E) = 0$. This structure also arises in the Hamiltonian studied in [19]. The function $\mathcal{F}(E)$ plays the role of the Jost function since its zeros gives the position of the bound states and its phase gives the scattering phase shift according to equation (4.31).

Before we continue with the general formalism it is worth studying a simple case which illustrates the results obtained so far.

### 4.1. An example: a quantum trap

Let us start with the classical version of a trap where a particle is restricted to the region $x_b < x < x_a$. The semiclassical number of states is given by the area formula (2.3),

$$n = \frac{A}{2\pi} = \int_{x_b}^{x_a} \frac{\mathrm{d}x}{2\pi} \frac{E}{x} = \frac{E}{2\pi} \log \frac{x_a}{x_b}, \tag{4.34}$$

which yields the eigenenergies

$$E_n = \frac{2\pi n}{\log(x_a/x_b)}, \qquad n \in \mathbb{N}. \tag{4.35}$$

The quantum version of this model is realized by two boundary states $\psi_{a,b}(x)$ proportional to delta functions, i.e.

$$\psi_a(x) = a_0 x_a^{1/2} \delta(x - x_a), \qquad \psi_b(x) = b_0 x_b^{1/2} \delta(x - x_b). \tag{4.36}$$

The associated potentials $a(q)$ and $b(q)$ are

$$\begin{aligned} &a(q) = a_0 \delta(q - q_a), \quad b(q) = b_0 \delta(q - q_b), \\ &q_a = \log x_a, \quad q_b = \log x_b. \end{aligned} \tag{4.37}$$

The various quantities defined above are readily computed obtaining

$$\begin{aligned} &\hat{a} = a_0 \mathrm{e}^{\mathrm{i}Eq_a}, \qquad \hat{b} = b_0 \mathrm{e}^{\mathrm{i}Eq_b}, \\ &S_{a,a} = \frac{a_0^2}{2}, \qquad S_{b,b} = \frac{b_0^2}{2}, \\ &S_{a,b} = a_0 b_0 \mathrm{e}^{\mathrm{i}Eq_{a,b}}, \qquad S_{b,a} = 0, \end{aligned} \tag{4.38}$$

where $q_{a,b} = q_a - q_b = \log(x_a/x_b)$. Plugging these equations into (4.25) yields

$$\mathcal{F}(E) = 1 + \left(\frac{a_0 b_0}{2}\right)^2 + a_0 b_0\, \mathrm{e}^{\mathrm{i}Eq_{a,b}}. \tag{4.39}$$

For generic values of $a_0$, $b_0$, the Jost function (4.39) never vanishes obtaining a spectrum which is continuous. However, $\mathcal{F}(E)$ vanishes provided the following condition holds

$$\epsilon \equiv \frac{a_0 b_0}{2} = \pm 1 \quad \Longrightarrow \quad \mathcal{F}(E) = 2(1 + \epsilon \mathrm{e}^{\mathrm{i}Eq_{a,b}}), \tag{4.40}$$

in which cases the spectrum contains bound states embbeded in the continuum with energies

$$\begin{aligned} &\text{if } \epsilon = 1 \quad \Longrightarrow \quad E_n = \frac{2\pi(n+1/2)}{q_{a,b}} \quad n \in \mathbb{N}, \\ &\text{if } \epsilon = -1 \quad \Longrightarrow \quad E_n = \frac{2\pi n}{q_{a,b}} \quad n \in \mathbb{N} \end{aligned} \tag{4.41}$$

that agree with the semiclassical energies (4.35) for $n \gg 1$. The un-normalized wavefunction of the bound states, i.e. $\mathcal{F}(E) = 0$, can be computed from equation (4.12)

$$\psi_E(x) = \frac{1}{x^{1/2-\mathrm{i}E}} \begin{cases} 1, & x_b < x < x_a, \\ 0, & x < x_b \text{ or } x > x_a, \end{cases} \tag{4.42}$$

which shows that they are confined to the region $(x_b, x_a)$. The wavefunctions when $\mathcal{F}(E) \neq 0$ can be similarly found obtaining

$$\psi_E(x) = \frac{1}{x^{1/2-\mathrm{i}E}} \begin{cases} \mathcal{F}(E), & 0 < x < x_b, \\ 1 - \left(\frac{a_0 b_0}{2}\right)^2, & x_b < x < x_a, \\ \mathcal{F}(-E), & x_a < x < \infty. \end{cases} \tag{4.43}$$

Hence if (4.40) holds, these wavefunctions vanish in the region $(x_b, x_a)$ which contains the trapped particles (4.42). In this example, the mechanism responsible for the existence of bound states is the transport of the particles from the position $x_a$ to the position $x_b$. At the quantum level the confinement requires the fine tuning of the couplings (see equation (4.40)) which introduces periodic or antiperiodic boundary conditions depending on the sign of $\epsilon$. When $|\epsilon| \neq 1$ the particle can escape the trap and the bound states become resonances.

## 5. Analyticity properties of $\mathcal{F}(E)$

As in ordinary quantum mechanics, the Jost function $\mathcal{F}(E)$ satisfies certain analyticity properties reflecting the causal structure of the dynamics. In our case, these properties follow from those of the function $S_{f,g}$ (equation (4.19)) and the definition (4.25).

Indeed, let us express $S_{f,g}(E)$ in terms of the Fourier transforms of the functions $f$, $g$. First, we replace $g(q)$ by its inverse Fourier transform

$$g(q') = \int_{-\infty}^{\infty} \frac{\mathrm{d}E'}{2\pi} \mathrm{e}^{\mathrm{i}Eq'}\, \hat{g}(-E') \tag{5.1}$$

back into equation (4.19), obtaining

$$S_{f,g}(E) = \int_{-\infty}^{\infty} \frac{\mathrm{d}E'}{2\pi} \hat{g}(-E') \int_{-\infty}^{\infty} \mathrm{d}q\, \mathrm{e}^{\mathrm{i}Eq} f(q) \int_{-\infty}^{q} \mathrm{d}q'\, \mathrm{e}^{\mathrm{i}(E'-E)q'}. \tag{5.2}$$

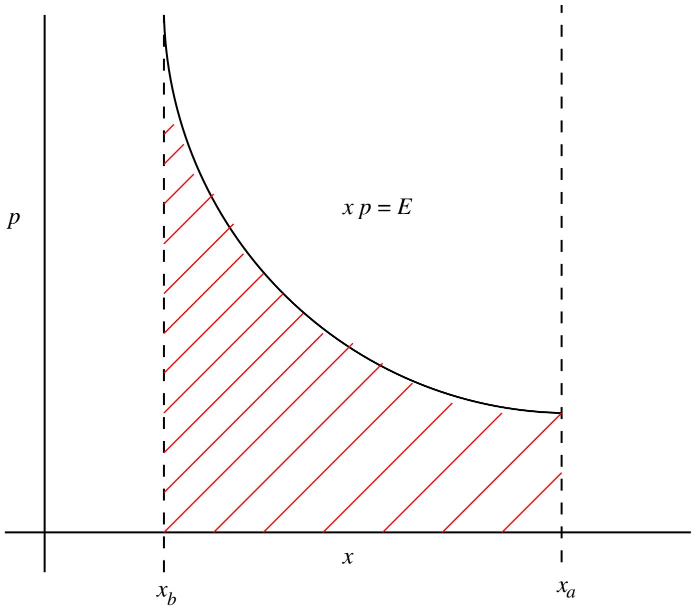


**Figure 4.** Semiclassical picture of the model represented by the potential (4.37).

The last integral is given by the distribution

$$\int_{-\infty}^{q} \mathrm{d}q' \, \mathrm{e}^{\mathrm{i}(E'-E)q'} = \mathrm{e}^{\mathrm{i}q(E'-E)} \left[ \pi \delta(E'-E) + \frac{1}{\mathrm{i}} P \, \frac{1}{E'-E} \right], \tag{5.3}$$

where $P$ denotes the Cauchy principal part. Plugging (5.3) into (5.2) and using the Fourier transform of $f$ gives,

$$S_{f,g}(E) = \frac{1}{2} \left[ \hat{f}(E)\, \hat{g}(-E) + P \int_{-\infty}^{\infty} \frac{\mathrm{d}E'}{\pi \mathrm{i}} \frac{\hat{f}(E')\, \hat{g}(-E')}{E'-E} \right]. \tag{5.4}$$

Alternatively, one can write (5.4) as

$$S_{f,g}(E) = \int_{-\infty}^{\infty} \frac{\mathrm{d}E'}{2\pi \mathrm{i}} \frac{\hat{f}(E')\, \hat{g}(-E')}{E'-E-\mathrm{i}\epsilon}, \tag{5.5}$$

with $\epsilon > 0$ an infinitesimal. Equation (5.5) shows that the poles of $S_{f,g}(E)$ are located in the lower half of the complex energy plane. Thus for well behave functions $\hat{f}, \hat{g}$, the function $S_{f,g}(E)$ will be analytic in the complex upper-half plane. These properties also apply to $\mathcal{F}(E)$ which is the product of $S_{f,g}$ functions with $f, g = a, b$. Another important property of the Jost function $\mathcal{F}(E)$ is that its zeros lie either on the real axis or below it, i.e.

$$\text{if } \mathcal{F}(E) = 0 \quad \Longrightarrow \quad \mathrm{Im}\, E \leqslant 0. \tag{5.6}$$

The proof of this equation is similar to the one done in [19], being convenient to regularize the interval $x \in (0, \infty)$ as $(N^{-1}, N)$ with $N \to \infty$.

In the appendix, we use the results obtained in this section to compute the norm of the eigenstates.

## 6. The quantum version of the BK model

Let us consider the BK constraints $x > l_x$ and $|p| > l_p$. It is rather natural to associate constraint $x > l_x$ with the wavefunction

$$\psi_b(x) = b_0\, l_x^{1/2}\, \delta(x - l_x), \tag{6.1}$$

which is localized at the boundary $x = l_x$. The factor $l_x^{1/2}$ gives the correct dimensionality to $\psi_b(x)$, with $b_0$ a dimensionless parameter. On the other hand the constraint $|p| > l_p$ admits two possible quantum versions,

$$\left\{ \begin{array}{l} \psi_a^+(x) \\ \psi_a^-(x) \end{array} \right. = 2a_0 \left( \frac{l_p}{2\pi} \right)^{1/2} \left\{ \begin{array}{l} \cos(l_p x), \\ \sin(l_p x). \end{array} \right. \tag{6.2}$$

Due to the fact that $\psi_a$ has to be real, one cannot choose a pure plane wave $\mathrm{e}^{\mathrm{i} l_p x}$. The boundary wavefunctions (6.1) and (6.2) are the cosine and sine Fourier transform of each other, namely

$$\left\{ \begin{array}{l} \psi_a^+(x) \\ \psi_a^-(x) \end{array} \right. = \frac{2a_0}{b_0} \left( \frac{l_p}{2\pi l_x} \right)^{1/2} \int_0^\infty \mathrm{d}y\ \psi_b(y) \left\{ \begin{array}{l} \cos(l_p x y / l_x), \\ \sin(l_p x y / l_x). \end{array} \right. \tag{6.3}$$

Indeed, extending the domain of $\psi_b(x)$ according to the parity of $\psi_a^\eta$ ($\eta = \pm$) one gets

$$\psi_b(-x) = \eta \psi_b(x) \quad \to \quad \psi_a^\eta(x) = \frac{a_0}{b_0} \left( \frac{l_p}{2\pi l_x} \right)^{1/2} \mathrm{e}^{\mathrm{i}(\pi/4)(\eta - 1)}\, \hat{\psi}_b \left( \frac{l_p x}{l_x} \right), \tag{6.4}$$

which are the quantum analogue of the classical equations (3.6). Later on, we shall consider more general wavefunctions $\psi_{a,b}$ to account for the fluctuations in the Riemann formula, imposing again equation (6.3). The relation (6.3) between $\psi_a^\pm$ and $\psi_b$ must imply a close link between their Mellin transforms $\hat{a}_\pm(E)$ and $\hat{b}(E)$. To derive it, let us write

$$\hat{a}_\pm(E) = \int_0^\infty x^{-1/2 + \mathrm{i}E}\ \psi_a^\pm(x) = \frac{2a_0}{b_0} \left( \frac{l_p}{2\pi l_x} \right)^{1/2} \int_0^\infty \mathrm{d}x\ x^{-1/2+\mathrm{i}E} \int_0^\infty \mathrm{d}y\ \psi_b(y) \left\{ \begin{array}{l} \cos(l_p x y / l_x), \\ \sin(l_p x y / l_x). \end{array} \right. \tag{6.5}$$

The basic integrals one needs are

$$\int_0^\infty \mathrm{d}x\ x^{-1/2+\mathrm{i}E} \left\{ \begin{array}{l} \cos(px) \\ \sin(px) \end{array} \right. = \frac{1}{2} \left( \frac{2\pi}{|p|} \right)^{(1/2)+\mathrm{i}E} \left\{ \begin{array}{l} \mathrm{e}^{2\mathrm{i}\theta_+(E)}, \\ \mathrm{e}^{2\mathrm{i}\theta_-(E)}, \end{array} \right. \tag{6.6}$$

where

$$\mathrm{e}^{2\mathrm{i}\theta_\pm(E)} = \left\{ \begin{array}{ll} \pi^{-\mathrm{i}E} \dfrac{\Gamma(1/4 + \mathrm{i}E/2)}{\Gamma(1/4 - \mathrm{i}E/2)}, & \eta = +, \\ \pi^{-\mathrm{i}E} \dfrac{\Gamma(3/4 + \mathrm{i}E/2)}{\Gamma(3/4 - \mathrm{i}E/2)}, & \eta = -. \end{array} \right. \tag{6.7}$$

The function $\theta_+(E)$ coincides with the phase of the Riemann zeta function (2.7), and more generally of the even Dirichlet L-functions, while $\theta_-(E)$ is the phase factor of the odd Dirichlet L-functions. These phases appear in the functional relation of even and odd L functions, and they arise in our context from the two possible relations between the boundary functions $\psi_a^\pm$ and $\psi_b$. Plugging equation (6.6) into (6.5) yields

$$\hat{a}_\pm(E) = \frac{a_0}{b_0} \left( \frac{2\pi l_x}{l_p} \right)^{\mathrm{i}E} \mathrm{e}^{2\mathrm{i}\theta_\pm(E)} \int_0^\infty \mathrm{d}y\ \psi_b(y) y^{-(1/2) - \mathrm{i}E}, \tag{6.8}$$

where the integral is nothing but $\hat{b}(-E)$, thus

$$\hat{a}_{\pm}(E) = \frac{a_0}{b_0}\left(\frac{2\pi l_x}{l_p}\right)^{\mathrm{i}E} \mathrm{e}^{2\mathrm{i}\theta_{\pm}(E)}\,\hat{b}(-E). \tag{6.9}$$

This important equation reflects the relation (6.3) which in turn is the quantum version of the $xp$ symmetry between boundaries. In the BK case, the Mellin transforms of the associated wavefunctions (6.1) and (6.2) are

$$\hat{a}_{\pm}(E) = a_0\left(\frac{2\pi}{l_p}\right)^{\mathrm{i}E} \mathrm{e}^{2\mathrm{i}\theta_{\pm}(E)}, \qquad \hat{b}(E) = b_0\, l_x^{\mathrm{i}E}, \tag{6.10}$$

which are pure phases, up to overall constants. The $S_{f,g}$ functions can be readily computed using equation (5.4). To do so, we first consider the products

$$\begin{aligned}
\hat{a}_{\pm}(E)\hat{a}_{\pm}(-E) &= a_0^2,\\
\hat{b}(E)\hat{b}(-E) &= b_0^2,\\
\hat{a}_{\pm}(E)\hat{b}(-E) &= a_0 b_0 \mathrm{e}^{2\mathrm{i}\theta_{\pm}(E)},\\
\hat{b}(E)\hat{a}_{\pm}(-E) &= a_0 b_0 \mathrm{e}^{-2\mathrm{i}\theta_{\pm}(E)},
\end{aligned} \tag{6.11}$$

where we used $l_x l_p = 2\pi$ and that $\theta_{\pm}(-E) = -\theta_{\pm}(E)$. The diagonal terms of $S_{f,g}$ are given simply by

$$S_{a_{\pm},a_{\pm}}(E) = \frac{a_0^2}{2}, \qquad S_{b,b}(E) = \frac{b_0^2}{2}, \tag{6.12}$$

since the Hilbert transform of a constant is zero, i.e.

$$P\int_{-\infty}^{\infty} \frac{\mathrm{d}t}{\pi\,\mathrm{i}}\frac{1}{t-E} = 0, \quad E \in \mathbb{R}. \tag{6.13}$$

The computation of $S_{a_{\pm},b}$ and $S_{b,a_{\pm}}$ uses the analytic properties of $\mathrm{e}^{2\mathrm{i}\theta_{\pm}(E)}$. Let us focus on the case of $\mathrm{e}^{2\mathrm{i}\theta_{+}(E)} = \mathrm{e}^{2\mathrm{i}\theta(E)}$. This function converges rapidly to zero as $|E| \to \infty$ in the upper half plane, and it has poles at $E_n = \mathrm{i}(2n + 1/2)$ $(n = 0, 1, \ldots)$ where it behaves like

$$\mathrm{e}^{2\mathrm{i}\theta(E)} \sim \frac{(-1)^n 2(2\pi)^{2n}}{(2n)!}\frac{1}{2n + 1/2 + \mathrm{i}E}. \tag{6.14}$$

We can split $\mathrm{e}^{2\mathrm{i}\theta(E)}$ into the sum

$$\mathrm{e}^{2\mathrm{i}\theta(E)} = \Omega_{+}(E) + \Omega_{-}(E), \qquad \Omega_{-}(E) = \sum_{n=0}^{\infty}\frac{(-1)^n\, 2(2\pi)^{2n}}{(2n)!}\frac{1}{2n + 1/2 + \mathrm{i}E}, \tag{6.15}$$

where $\Omega_{+}(E)$ is analytic in the upper half plane and goes to zero at $+\mathrm{i}\infty$, while $\Omega_{-}(E)$ has poles in the upper half plane and behaves as $1/E$ at infinity. The function $\Omega_{-}(E)$ can also be written as

$$\Omega_{-}(E) = 2\int_0^1 \mathrm{d}x\; x^{-1/2+\mathrm{i}E}\cos(2\pi x) = \frac{4}{1+2\mathrm{i}E}\;{}_1F_2\left(\frac{1}{4}+\mathrm{i}\frac{E}{2}, \frac{1}{2}, \frac{5}{4}+\mathrm{i}\frac{E}{2}, -\pi^2\right), \tag{6.16}$$

where ${}_1F_2$ is a hypergeometric function of the type (1,2). From the analyticity properties of $\Omega_{\pm}$ one gets immediately their Hilbert transform

$$P\int_{-\infty}^{\infty}\frac{\mathrm{d}t}{\pi\,\mathrm{i}}\frac{\Omega_{\pm}(t)}{t-E} = \pm\,\Omega_{\pm}(E), \quad E \in \mathbb{R}. \tag{6.17}$$

Hence $S_{a_+,b} \equiv S_{a,b}$, as given by equation (5.4), becomes

$$S_{a,b}(E) = \frac{a_0 b_0}{2}\left[ e^{2i\theta(E)} + P\int_{-\infty}^{\infty} \frac{dt}{\pi i}\frac{e^{2i\theta(t)}}{t-E} \right]$$
$$= \frac{a_0 b_0}{2}\left[\Omega_+(E) + \Omega_-(E) + \Omega_+(E) - \Omega_-(E)\right]$$
$$= a_0 b_0\, \Omega_+(E). \tag{6.18}$$

Similarly one finds

$$S_{b,a}(E) = a_0 b_0\, \Omega_-(-E). \tag{6.19}$$

Notice that both functions are analytic in the upper half plane. The Jost function finally reads

$$\mathcal{F}(E) = 1 + a_0 b_0(\Omega_+(E) - \Omega_-(-E)) + \left(\frac{a_0 b_0}{2}\right)^2 - (a_0 b_0)^2 \Omega_+(E)\Omega_-(-E). \tag{6.20}$$

In the asymptotic limit $|E| \gg 1$

$$\Omega_-(E) \sim \frac{1}{E} \rightarrow \Omega_+(E) = e^{2i\theta(E)} + O\left(\frac{1}{E}\right), \tag{6.21}$$

which implies

$$\mathcal{F}(E) = 1 + a_0 b_0\, e^{2i\theta(E)} + \left(\frac{a_0 b_0}{2}\right)^2 + O\left(\frac{1}{E}\right). \tag{6.22}$$

This Jost function has zeros on the real axis, up to order $1/E$, provided

$$\epsilon = \frac{a_0 b_0}{2} = \pm 1 \quad \Longrightarrow \quad \mathcal{F}(E) = 2(1 + \epsilon e^{2i\theta(E)}) + O\left(\frac{1}{E}\right). \tag{6.23}$$

The choice $\epsilon = -1$ reproduces the smooth part of the Riemann formula (2.6) since,

$$\epsilon = -1 \quad \Longrightarrow \quad 1 - e^{2i\theta(E)} = 1 - e^{2\pi i\langle \mathcal{N}(E)\rangle} = 0, \tag{6.24}$$

where $E$ is the average position of the zeros. On the other hand the choice $\epsilon = 1$ leads to

$$\epsilon = 1 \quad \Longrightarrow \quad 1 + e^{2i\theta(E)} = 0 \quad \Longrightarrow \quad \cos\theta(E) = 0 \tag{6.25}$$

so that the number of zeros in the interval $(0, E)$ is given by

$$\mathcal{N}_{\rm sm}(E) = \frac{\theta(E)}{\pi} + \frac{3}{2}, \tag{6.26}$$

which gives a better numerical approximation than the term $\langle \mathcal{N}(E)\rangle$ that appears in the exact Riemann formula (2.6) (see also figure 2). In the case of the sine boundary function (6.2) one similarly obtains the smooth part of the zeros of the odd Dirichlet L-functions.

In summary, we have shown that the semiclassical BK boundary conditions have a quantum counterpart in terms of the boundary wavefunctions $\psi_{a,b}$, and that the average Riemann zeros become asymptotically bound states of the model or more appropiately resonances.

## 7. The quantum model of the Riemann zeros

In section 3, we showed how to incorporate the fluctuations of the energy levels in the heuristic $xp$ model by means of the functions $p_{\rm cl}(x)$ and $x_{\rm cl}(p)$ which define the boundaries of the allowed phase space. These functions are given by equation (3.15) in terms of the density of the fluctuation part of the energy levels. The relation between the wavefunctions $\psi_a$ and $\psi_b$ and the boundary wavefunctions $p_{\rm cl}(x)$ and $x_{\rm cl}(p)$ is given by the following conditions:

$$\left(\log \frac{|\hat{p}|}{l_p} + \pi n'_{\rm fl}(H_0)\right) |\psi_a\rangle = 0, \tag{7.1}$$

$$\left(\log \frac{\hat{x}}{l_x} + \pi n'_{\rm fl}(H_0)\right) |\psi_b\rangle = 0, \tag{7.2}$$

where $n'_{\rm fl}(E) = {\rm d}n_{\rm fl}(E)/{\rm d}E$ and $H_0$ is the non interacting Hamiltonian (4.1). The hat over $x$ and $p$ stress the fact that they are operators. To solve these equations let us write them as

$$(\log |\hat{p}| + \lambda_{\rm p} + \pi n'_{\rm fl}(H_0))|\psi_a\rangle = 0, \tag{7.3}$$

$$(\log \hat{x} + \lambda_x + \pi n'_{\rm fl}(H_0))|\psi_b\rangle = 0, \tag{7.4}$$

$$\lambda_p = -\log l_p, \qquad \lambda_x = -\log l_x. \tag{7.5}$$

It is convenient to expand the states $|\psi_{a,b}\rangle$ in the basis (4.3)

$$|\psi_{a,b}\rangle = \int_{-\infty}^{\infty} {\rm d}E\, \psi_{a,b}(E)|\phi_E\rangle, \qquad \langle x|\phi_E\rangle = \frac{1}{\sqrt{2\pi}} \frac{1}{x^{1/2-{\rm i}E}}. \tag{7.6}$$

Let us first consider equation (7.4) which in the basis (7.6) becomes

$$\int_{-\infty}^{\infty} {\rm d}E' \langle\phi_E| \log \hat{x} |\phi_{E'}\rangle \psi_b(E') + (\lambda_x + \pi n'_{\rm fl}(E))\psi_b(E) = 0. \tag{7.7}$$

The matrix elements of the operator $\log \hat{x}$ can be readily computed,

$$\langle\phi_E| \log \hat{x} |\phi_{E'}\rangle = -{\rm i}\delta'(E' - E), \tag{7.8}$$

which substituted into (7.7) and upon integration yields

$${\rm i}\frac{{\rm d}\psi_b(E)}{{\rm d}E} + (\lambda_x + \pi n'_{\rm fl}(E))\psi_b(E) = 0. \tag{7.9}$$

The solution of (7.9) is simply

$$\psi_b(E) = \psi_{b,0}\, {\rm e}^{{\rm i}(\lambda_x E + \pi n_{\rm fl}(E))}, \tag{7.10}$$

where $\psi_{b,0}$ is an integration constant. The $x$-space representation of $\psi_b$ follows from (7.10) and (7.6)

$$\psi_b(x) = \int_{-\infty}^{\infty} {\rm d}E\, \psi_b(E)\phi_E(x) = \psi_{b,0} \int_{-\infty}^{\infty} \frac{{\rm d}E}{\sqrt{2\pi}} {\rm e}^{{\rm i}(\lambda_x E + \pi n_{\rm fl}(E))} x^{-1/2+{\rm i}E}. \tag{7.11}$$

Recalling that $\psi_b(x) = b(x)/\sqrt{x}$ one gets

$$b(x) = \psi_{b,0} \int_{-\infty}^{\infty} \frac{{\rm d}E}{\sqrt{2\pi}} {\rm e}^{{\rm i}(\lambda_x E + \pi n_{\rm fl}(E))} x^{{\rm i}E}. \tag{7.12}$$

Observing that $b(x)$ is related to its Fourier transform $\hat{b}(E)$, as

$$b(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{2\pi} \hat{b}(E) x^{-\mathrm{i}E}, \tag{7.13}$$

one finally obtains

$$\hat{b}(E) = \sqrt{2\pi}\, \psi_{b,0} \mathrm{e}^{-\mathrm{i}(\lambda_x E + \pi n_{\mathrm{fl}}(E))}, \tag{7.14}$$

where we assumed that $n_{\mathrm{fl}}(E)$ is an odd function of $E$. If $n_{\mathrm{fl}}(E) = 0$, equation (7.14) reproduces (6.10), i.e.

$$n_{\mathrm{fl}}(E) = 0 \quad \Longrightarrow \quad \hat{b}(E) = \sqrt{2\pi}\, \psi_{b,0} l_x^{\mathrm{i}E} = b_0 l_x^{\mathrm{i}E}. \tag{7.15}$$

To simplify the notations we shall write (7.14) as

$$\hat{b}(E) = b_0 l_x^{\mathrm{i}E}\, \mathrm{e}^{-\mathrm{i}\pi n_{\mathrm{fl}}(E)}. \tag{7.16}$$

Let us now solve the condition (7.3) for the wavefunction $\psi_a$. We first need to define the operator $\log|\hat{p}|$ acting in the Hilbert space expanded by the functions $\phi_E (E \in \mathbb{R})$. In this respect it is worth remembering that the operator $\hat{p} = -\mathrm{i}\,\mathrm{d}/\mathrm{d}x$ is self-adjoint in the real line $(-\infty, \infty)$ and in the finite intervals $(a, b)$, but not in the half-line $(0, \infty)$ [28]. However, the operator $\hat{p}^2$ admits infinitely many self-adjoint extensions in the half-line provide the wavefunctions satisfy the boundary condition

$$\psi'(0) = \kappa\, \psi(0), \tag{7.17}$$

where $\kappa \in \mathbb{R} \cup \infty$. We shall confine ourselves to the cases where $\kappa = 0$ and $\infty$, which correspond to the von Neumann and Dirichlet BCs, respectively,

$$\begin{aligned} \kappa &= 0 \rightarrow \psi'(0) = 0, \\ \kappa &= \infty \rightarrow \psi(0) = 0. \end{aligned} \tag{7.18}$$

The corresponding eigenstates of the operator $\hat{p}^2$ with eigenvalues $p^2$ read

$$\left\{ \begin{array}{c} \chi_p^+ \\ \chi_p^- \end{array} \right. = \sqrt{\frac{2}{\pi}} \left\{ \begin{array}{ll} \cos(px) & (p > 0), \\ \sin(px) & (p > 0). \end{array} \right. \tag{7.19}$$

These bases are complete in the space of functions defined in $(x > 0)$, i.e.

$$\int_0^{\infty} \mathrm{d}p (\chi_p^{\eta}(x))^* \chi_p^{\eta}(x') = \delta(x - x'), \quad x, x' > 0, \quad \eta = \pm. \tag{7.20}$$

The operator $\log|\hat{p}|$ will be defined as $\frac{1}{2}\log \hat{p}^2$, and therefore admits the same self-adjoint extensions as $\hat{p}^2$. The analogue of equation (7.7) reads now

$$\int_{-\infty}^{\infty} \mathrm{d}E' \langle \phi_E | \log|\hat{p}| |\phi_{E'}\rangle \psi_a(E') + (\lambda_{\mathrm{p}} + \pi n'_{\mathrm{fl}}(E)) \psi_a(E) = 0. \tag{7.21}$$

The matrix elements of $\log|\hat{p}|$ can be computed introducing the resolution of the identity in the basis (7.19),

$$\langle \phi_E | \log|\hat{p}| |\phi_{E'}\rangle = \int_0^{\infty} \mathrm{d}p \log p \langle \phi_E | \chi_p^{\eta}\rangle \langle \chi_p^{\eta} | \phi_{E'}\rangle, \tag{7.22}$$

where the overlap of the eigenstates of $\hat{p}^2$ and $H_0$ are

$$\langle \chi_p^{\pm} | \phi_E \rangle = \int_0^{\infty} \frac{\mathrm{d}x}{\pi} x^{-(1/2)+\mathrm{i}E} \begin{cases} \cos(px), \\ \sin(px). \end{cases} \tag{7.23}$$

These integrals were already computed in equation (6.6), and the result is

$$\langle \chi_p^{\pm} | \phi_E \rangle = \frac{(2\pi)^{-1/2+\mathrm{i}E}}{p^{1/2+\mathrm{i}E}} \mathrm{e}^{2\mathrm{i}\theta_{\pm}(E)}. \tag{7.24}$$

Plugging this equation into (7.22), and performing the integral gives

$$\langle \phi_E | \log |\hat{p}| | \phi_{E'} \rangle = \mathrm{i}\delta'(E' - E)(2\pi)^{\mathrm{i}(E'-E)} \mathrm{e}^{2\mathrm{i}(\theta_\eta(E') - \theta_\eta(E))}, \tag{7.25}$$

which introduced into (7.21) yields a differential equation whose solution is

$$\psi_{a_\eta}(E) = \psi_{a,0} (2\pi)^{-\mathrm{i}E} \mathrm{e}^{-\mathrm{i}(\lambda_{\mathrm{p}} E + \pi n_{\mathrm{fl}}(E) + 2\theta_\eta(E))}. \tag{7.26}$$

The function $\psi_a(x)$ reads

$$\psi_{a_\eta}(x) = \int_{-\infty}^{\infty} \mathrm{d}E\, \psi_{a_\eta}(E) \phi_E(x) = \psi_{a,0} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{\sqrt{2\pi}} (2\pi)^{-\mathrm{i}E} \mathrm{e}^{-\mathrm{i}(\lambda_{\mathrm{p}} E + \pi n_{\mathrm{fl}}(E) + 2\theta_\eta(E))} x^{-1/2+\mathrm{i}E}, \tag{7.27}$$

while

$$a_\eta(x) = \psi_{a,0} \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{\sqrt{2\pi}} (2\pi)^{-\mathrm{i}E} \mathrm{e}^{-\mathrm{i}(\lambda_{\mathrm{p}} E + \pi n_{\mathrm{fl}}(E) + 2\theta_\eta(E))} x^{\mathrm{i}E}, \tag{7.28}$$

whose Fourier transform is

$$\hat{a}_\eta(E) = \psi_{a,0} (2\pi)^{1/2+\mathrm{i}E} \mathrm{e}^{\mathrm{i}(\lambda_{\mathrm{p}} E + \pi n_{\mathrm{fl}}(E) + 2\theta_\eta(E))}. \tag{7.29}$$

If there are no fluctuations, equation (7.29) reduces to

$$n_{\mathrm{fl}}(E) = 0 \quad \Longrightarrow \quad \hat{a}_\eta(E) = \sqrt{2\pi}\, \psi_{a,0} \left( \frac{2\pi}{l_p} \right)^{\mathrm{i}E} \mathrm{e}^{2\mathrm{i}\theta_\eta(E)}, \tag{7.30}$$

which coincides with equation (6.10). To simplify notations we shall write (7.29) as

$$\hat{a}_\eta(E) = a_0 \left( \frac{2\pi}{l_p} \right)^{\mathrm{i}E} \mathrm{e}^{\mathrm{i}(\pi n_{\mathrm{fl}}(E) + 2\theta_\eta(E))}. \tag{7.31}$$

The two solutions (7.16) and (7.31) satisfy the duality relation (6.9) and hence the wavefunctions $\psi_{a_\pm}(x)$ is the cosine or sine Fourier transform of $\psi_b(x)$ (see equation (6.3)).

Having found the boundary wavefunctions for generic fluctuations we turn into the computation of the corresponding Jost function. The basic products of the $\hat{a}$ and $\hat{b}$ functions needed to find the $S_{f,g}$ functions are similar to equation (6.11),

$$\begin{aligned} \hat{a}_{\pm}(E)\hat{a}_{\pm}(-E) &= a_0^2, \\ \hat{b}(E)\hat{b}(-E) &= b_0^2, \\ \hat{a}_{\pm}(E)\hat{b}(-E) &= a_0 b_0\, \mathrm{e}^{2\mathrm{i}(\theta_{\pm}(E) + \pi n_{\mathrm{fl}}(E))}, \\ \hat{b}(E)\hat{a}_{\pm}(-E) &= a_0 b_0\, \mathrm{e}^{-2\mathrm{i}(\theta_{\pm}(E) + \pi n_{\mathrm{fl}}(E))}. \end{aligned} \tag{7.32}$$

The diagonal terms of $S_{f,g}$ are the same as in equation (6.12), i.e.

$$S_{a_\pm, a_\pm}(E) = \frac{a_0^2}{2}, \qquad S_{b,b}(E) = \frac{b_0^2}{2}, \tag{7.33}$$

while the evaluation of the off-diagonal terms depends on the analytic properties of the function $e^{2\pi i n_\pm(E)}$ where

$$n_\pm(E) \equiv \frac{\theta_\pm(E)}{\pi} + n_{\rm fl}(E). \tag{7.34}$$

This definition is strongly reminiscent of the Riemann formula (2.6), with $n_\pm(E)$ playing the role of $\mathcal{N}_{\rm R}(E)$, and $n_{\rm fl}(E)$ that of $\mathcal{N}_{\rm fl}(E)$. However, we must keep in mind that $\mathcal{N}_{\rm R}(E)$ is a step function while we expect $n_\pm(E)$ to be a continuous interpolating function between the zeros. The value of $S_{a_\pm,b}$ is given by the integral

$$S_{a_\pm,b}(E) = \frac{a_0 b_0}{2}\left[e^{2\pi i n_\pm(E)} + P\int_{-\infty}^{\infty}\frac{dt}{\pi i}\frac{e^{2\pi i n_\pm(t)}}{t-E}\right]. \tag{7.35}$$

We shall make the asumption that $e^{2\pi i n_\pm(E)}$ is an analytic function in the upper half plane which goes to zero as $|E| \to \infty$. In this case the Cauchy integral on the RHS of (7.35) is equal to $e^{2\pi i n_\pm(E)}$ and one finds

$$S_{a_\pm,b}(E) = a_0 b_0\, e^{2\pi i n_\pm(E)}. \tag{7.36}$$

Similarly $S_{b,a_\pm}$ vanishes so that the Jost function reduces to

$$\mathcal{F}(E) = 1 + a_0 b_0\, e^{2\pi i n_\pm(E)} + \left(\frac{a_0 b_0}{2}\right)^2 \tag{7.37}$$

and under the usual choice

$$\epsilon = \frac{a_0 b_0}{2} = \pm 1 \quad \Longrightarrow \quad \mathcal{F}(E) = 2(1 + \epsilon e^{2\pi i n_\pm(E)}). \tag{7.38}$$

When $n_{\rm fl} = 0$ the results of the previous subsection showed that $\epsilon = 1$ gives a better numerical estimate to the smooth part of the zeros. In the following we shall also make that choice which implies that the number of zeros of $\mathcal{F}(E)$ in the interval $(0, E)$ is

$$\mathcal{N}_{\rm QM}(E) = \mathcal{N}_{\rm sm}(E) + n_{\rm fl}(E) = n_\pm(E) + \tfrac{3}{2}, \tag{7.39}$$

where $\mathcal{N}_{\rm sm}(E)$ was defined in (6.26) for the particular case of the zeta function $\zeta(s)$, which corresponds to $n_+(E)$. Equation (7.39) agrees asymptotically with the semiclassical formula (3.12), which confirms the ansatz made for the states $\psi_a$ and $\psi_b$.

### 7.1. The connection with the Riemann–Siegel formula

The next problem is to find the function $n_{\rm fl}(E)$, and therefore $\mathcal{N}_{\rm QM}(E)$, which gives the exact location of the Riemann zeros. Let us consider the case of the zeta function with the following choices of parameters:

$$\eta = +, \quad \epsilon = 1, \quad a_0 = b_0 = \sqrt{2}, \quad l_x = 1, \quad l_p = 2\pi \tag{7.40}$$

which correspond to the potentials (recall (7.31) and (7.16))

$$\begin{aligned} \hat{a}(t) &= e^{i(2\theta(t) + \pi n_{\rm fl}(t))} = e^{i(\theta(t) + \pi n(t))}, \\ \hat{b}(t) &= e^{-i\pi n_{\rm fl}(t))} = e^{i(\theta(t) - \pi n(t))}, \end{aligned} \tag{7.41}$$

where we skip a common factor $\sqrt{2}$ and denote $n(E) \equiv n_+(E)$. These two functions are interchanged under the transformation

$$\begin{aligned} \hat{a}(t) &\to e^{2i\theta(t)}\hat{a}(-t) = \hat{b}(t), \\ \hat{b}(t) &\to e^{2i\theta(t)}\hat{b}(-t) = \hat{a}(t), \end{aligned} \tag{7.42}$$

so that their sum is left invariant,

$$\hat{a}(t) + \hat{b}(t) \to e^{2i\theta(t)}(\hat{a}(-t) + \hat{b}(-t)) = \hat{a}(t) + \hat{b}(t). \tag{7.43}$$

The functional relation satisfied by the zeta function implies

$$\zeta(1/2 - it) \to e^{2i\theta(t)}\zeta(1/2 + it) = \zeta(1/2 - it). \tag{7.44}$$

which suggests to relate $\hat{a} + \hat{b}$ and $\zeta$ as

$$\zeta(1/2 - it) = \rho(t)(\hat{a}(t) + \hat{b}(t)), \tag{7.45}$$

where $\rho(t)$ is a proportionally factor. Using equations (7.42) in (7.45) yields

$$\zeta(1/2 - it) = 2\rho(t)e^{i\theta(t)}\cos(\pi n(t)). \tag{7.46}$$

This formula can be compared with the parametrization of the zeta function in terms of the Riemann–Siegel zeta function $Z(t)$ and its phase $\theta(t)$,

$$\zeta(1/2 - it) = Z(t)e^{i\theta(t)}, \tag{7.47}$$

which leads to,

$$Z(t) = 2\rho(t)\cos(\pi n(t)). \tag{7.48}$$

This equation is rather interesting since it implies that the zeros of $\cos(\pi n(t))$, which give the bound states of the QM model, are also zeros of $Z(t)$, of course if $\rho(t)$ does not have poles at those values. Vice versa, the zeros of $Z(t)$ can be zeros either of $\cos(\pi n(t))$, or of $\rho(t)$, or both. The latter possibility would be absent if the Rieman zeros are simple, as is expected to be the case.

A first hint on the structure of the functions $\rho(t)$ and $\cos(\pi n(t))$ can be obtained using the Riemann–Siegel formula for $Z(t)$,

$$Z(t) = 2\sum_{n=1}^{\nu(t)} n^{-1/2}\cos(\theta(t) - t\log n) + R(t), \qquad \nu(t) = \left[\sqrt{\frac{t}{2\pi}}\right], \tag{7.49}$$

where $[x]$ is the integer part of $x$ and $R(t)$ is a remainder of order $t^{-1/4}$. Combining the last two equations one finds

$$\begin{aligned} Z(t) &= 2\rho(t)\left[\cos\theta(t)\cos(\pi n_{\text{fl}}(t)) - \sin\theta(t)\sin(\pi n_{\text{fl}}(t))\right] \\ &\sim 2\left[\cos\theta(t)\sum_{n=1}^{\nu(t)}\frac{\cos(t\log n)}{n^{1/2}} + \sin\theta(t)\sum_{n=1}^{\nu(t)}\frac{\sin(t\log n)}{n^{1/2}}\right], \end{aligned} \tag{7.50}$$

which suggests the following identifications

$$\begin{aligned} \rho(t)\cos(\pi n_{\text{fl}}(t)) &\sim \sum_{n=1}^{\nu(t)}\frac{\cos(t\log n)}{n^{1/2}}, \\ \rho(t)\sin(\pi n_{\text{fl}}(t)) &\sim -\sum_{n=1}^{\nu(t)}\frac{\sin(t\log n)}{n^{1/2}} \end{aligned} \tag{7.51}$$

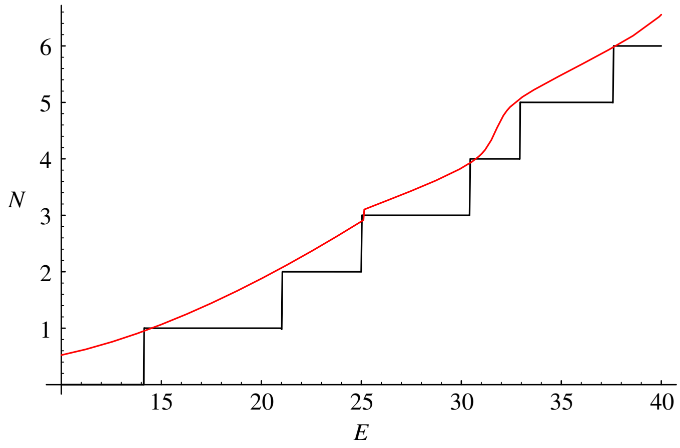


**Figure 5.** In black: $\mathcal{N}_\mathrm{R}(E)$, in red: $\mathcal{N}_\mathrm{QM}(E)$ in the interval (10, 40).

that can be combined into

$$f(t) \equiv \rho(t) \mathrm{e}^{\mathrm{i}\pi n_\mathrm{fl}(t)} \sim \sum_{n=1}^{\nu(t)} \frac{1}{n^{1/2+\mathrm{i}t}}. \tag{7.52}$$

The fluctuation function $n_\mathrm{fl}(t)$ is then given by the phase of $f(t)$, i.e.

$$n_\mathrm{fl}(t) = \frac{1}{\pi} \mathrm{Im} \log f(t). \tag{7.53}$$

In figure 5, we plot the values of $\mathcal{N}_\mathrm{QM}(t)$ that correspond to the approximate formula (7.52), which shows an excellent agreement with the Riemann formula (2.6). This is expected from the fact that the main term of the Riemann–Siegel formula already gives accurate results for the lowest Riemann zeros. For higher zeros one has to compute more terms of the remainder $R(t)$ depending on the desired accuracy. Observe that $\mathcal{N}_\mathrm{QM}(t)$ is a smooth function, except for some jumps at higher values of $t$ (not shown in figure 5) due to the approximation made, unlike $\mathcal{N}_\mathrm{R}(t)$, which is a step function.

In figure 6, we plot the values of (7.53) together with those of the fluctuation part of the Riemann formula (2.6), i.e.

$$\mathcal{N}_\mathrm{fl}(t) = \frac{1}{\pi} \mathrm{Im} \log \zeta \left(\tfrac{1}{2} + \mathrm{i}t\right). \tag{7.54}$$

The jumps in $\mathcal{N}_\mathrm{fl}(t)$ correspond to the Riemann zeros, while those of $n_\mathrm{fl}(t)$ correspond, either to jumps of the function $\nu(t)$ appearing in the Riemann Siegel formula (7.49), or to those points where the curve $f(t)$ cuts the negative real axis in the complex plane.

We gave in section 2 a formal expression of equation (7.54) in terms of prime numbers, equation (2.10), which resembles the fluctuation part (2.11) of a quantum chaotic system. Equation (2.10) is based on the Euler product formula (2.9) which is not valid in the case where $s = 1/2 + \mathrm{i}t$, since $\mathrm{Re}\, s > 1$ for convergence of the infinite product. The Euler product formula does not apply to the truncated sum (7.52), however we shall naively try to establish a relationship. Let us denote by $p_n$ the $n$th-prime number, e.g. $p_1 = 2$, $p_2 = 3$, etc, and by $\Pi(x)$ the number of primes less than or equal to $x$. The sum (7.52) involves all integers up to $\nu(t)$, which can be expressed as products of the first $\mu(t)$ prime numbers where

$$\mu(t) = \Pi(\nu(t)), \qquad p_{\mu(t)} = \inf\{p\} < \nu(t). \tag{7.55}$$

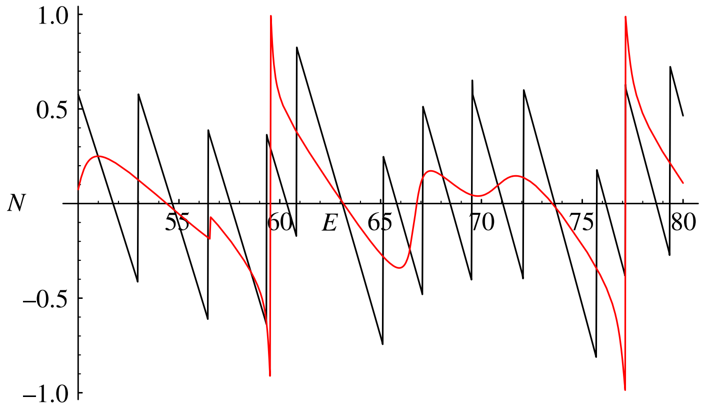


**Figure 6.** In black: $\mathcal{N}_{\rm fl}(E)$, in red: $n_{\rm fl}(E)$ in the interval (50, 80).

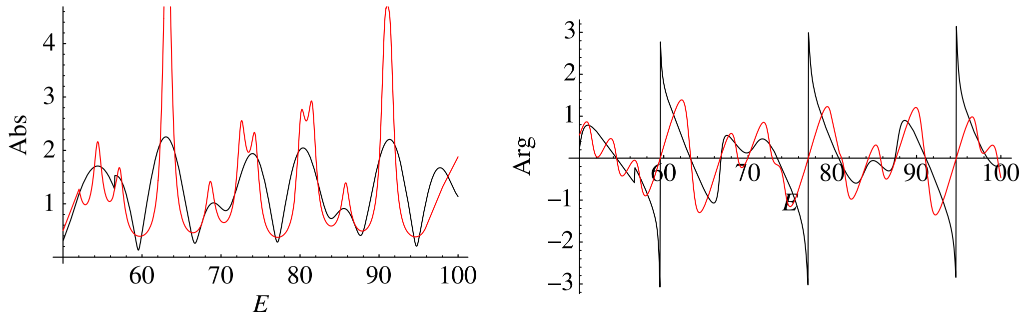


**Figure 7.** Left: in black: $|f(E)|$, in red: $|\zeta_{\rm E}(1/2+{\rm i}E)|$ in the interval (50, 100). Right: in black: Arg $f(E)$, in red: Arg $\zeta_{\rm E}(1/2+{\rm i}E)$.

Using these functions we define a truncated Euler product as

$$\zeta_{\rm E}(1/2+{\rm i}t) \equiv \prod_{n=1}^{\mu(t)} \frac{1}{1-p_n^{-1/2-{\rm i}t}}. \tag{7.56}$$

It is easy to see that $\zeta_{\rm E}(1/2+{\rm i}t)$ is not equal to $f(t)$, for there are terms in (7.56) which do not appear in (7.52), although all the terms appearing in the latter sum also appear in the former product. The point is that a numerical comparison of these two functions shows a qualitative agreement as depicted in figure 7. Indeed, the minima and maxima of their absolute value are located around the same points, and the same happens for the zeros of their arguments. The conclusion we draw from these heuristic considerations is that the function $f(t)$ contains some sort of information related to the prime numbers although not in the form of an Euler product formula as is the case of $\zeta_{\rm E}(1/2+{\rm i}t)$. It would be interesting to investigate the consequences of this result from the point of view of quantum chaos.

### *7.2. The BK formula of $Z(t)$*

The main term of the Riemann–Siegel formula (7.49) is not analytic in $t$ due to the discontinuity in the main sum. This problem was solved by Berry and Keating who found an alternative expression for $Z(t)$ [29]. The formula is

$$Z(t) = \sum_{n=1}^{\infty} (T_n(t) + T_n(-t)), \tag{7.57}$$

where

$$\begin{aligned} T_n(t) &= T_n^*(-t) = \frac{e^{i\theta(t)}}{n^{1/2+it}} \beta_n(t), \\ \beta_n(t) &= \frac{1}{2\pi i} \int_{C_-} \frac{dz}{z} e^{-z^2 K^2/(2|t|)} e^{i[\theta(z+t)-\theta(t)-z\log n]} \end{aligned} \tag{7.58}$$

and $C_-$ is an integration contour in the lower half plane with Im $< -1/2$ that avoids a cut starting at the branch point $z = -t - i/2$. The constant $K$ in (7.58) can be chosen at will and it is related to the number of terms of the RS formula that has been smoothed for large values of $t$. Using equation (7.57) one can write the zeta function as

$$\zeta(1/2 - it) = e^{2i\theta(t)} \sum_{n=1}^{\infty} \frac{\beta_n(t)}{n^{1/2+it}} + \sum_{n=1}^{\infty} \frac{\beta_n(-t)}{n^{1/2-it}}, \tag{7.59}$$

which can be compared with (7.45) obtaining

$$f(t) = \rho(t) e^{i\pi n_{fl}(t)} = \sum_{n=1}^{\infty} \frac{\beta_n(t)}{n^{1/2+it}} \tag{7.60}$$

so that (7.59) can be written as

$$\zeta(1/2 - it) = e^{2i\theta(t)} f(t) + f(-t). \tag{7.61}$$

Equation (7.60) gives an exact expression of $f(t)$, which is, in fact, a smooth version of (7.52). BK also found a series for $Z(t)$ which improves the RS series. The first term of that series corresponds to the following value of the $\beta_n(t)$ functions

$$\begin{aligned} &\beta_n^{(0)}(t) = \tfrac{1}{2}\mathrm{Erfc}\left( \frac{\xi(n,t)}{Q(K,t)} \sqrt{t/2} \right), \\ &\xi(n,t) = \log n - \theta'(t), \qquad Q^2(K,t) = K^2 - it\theta''(t), \end{aligned} \tag{7.62}$$

where Erfc is the complementary error function. Using these formulae one can find a better numerical evaluation of the functions $\mathcal{N}_{QM}(t)$ and $n_{fl}(t)$.

It is perhaps worth mentioning that equation (7.61), with the approximate value of $f(t)$ given by (7.52), is a particular case of the so-called approximate functional relation due to Hardy and Littlewood [1, 2]

$$\zeta(s) = \sum_{n \leqslant x} n^{-s} + \pi^{s-1/2} \frac{\Gamma((1-s)/2)}{\Gamma(s/2)} \sum_{n \leqslant y} n^{1-s} + O(x^{-\sigma}) + O(|t|^{1/2-\sigma} y^{\sigma-1}), \tag{7.63}$$

where $s = \sigma + it$, $|t| = 2\pi xy$, $0 < \sigma < 1$. Recalling that in our model $t$ is the energy $E$, then equation $|t| = 2\pi xy$ becomes the hyperbola $|E| = xp$ with $p = 2\pi y = l_p y$ so that the sums in (7.63) run over the integer values of the positions and momenta in units of $l_x$ and $l_p$, respectively. Equation (7.63) also suggests that the case where $\sigma \neq 1/2$ could be related to the non hermitean Hamiltonian $H_0 = (xp + px)/2 - i(\sigma - 1/2)$ whose right (resp. left) eigenfunctions are given by $1/x^{\sigma - iE}$ (resp. $1/x^{1-\sigma-iE}$).

On more general grounds, we would like to mention two important points. Firstly, one still needs to show that the function $n(t)$, defined in equation (7.34), is such that $e^{2\pi i n(t)}$ is analytic in the upper-half plane and that it goes to zero as $|t| \to \infty$, so that the Jost function is indeed given by equation (7.39), as we have assumed so far. Secondly, and related to the latter point, the function $n_{fl}(t)$ is well defined provided $f(t)$ does not vanish for $t$ real, in which case (7.61) also reads

$$\zeta(1/2 - it) = f(-t)\left(1 + e^{2i\theta(t)} \frac{f(t)}{f(-t)}\right) = f(-t)\mathcal{F}(t), \tag{7.64}$$

which shows that our construction of a QM model of the Riemann zeros relies on the absence of zeros of the function $f(t)$ on the critical line. These zeros were investigated by Bombieri long ago in an attempt to improve the existing lower bounds for the number of Riemann zeros on the critical line [30]. In this regard our results give further support to, but not proof of, the RH. As suggested in [19, 20] that proof would follow if the zeta function $\zeta(1/2 - it)$ can be realized as the Jost function of a QM model of the sort discussed so far, due to its special analyticity properties. Equation (7.64) gives a partial realization of this idea but the function $f(t)$ lacks a physical interpretation so far. The latter approach is analogous to the ones proposed in the past by several authors where the zeta function gives the scattering phase shift of some quantum mechanical model, particularly on the line $\mathrm{Re}\, s = 1$ [31]–[39].

Another important question is: where are the prime numbers in our construction? As suggested by the quantum chaos scenario, the prime numbers may well be classical objects hidden in the quantum model, so the next question is: what is the classical limit of the Hamiltonian? The free part is of course given by $xp$, but the interacting part is an antisymmetric matrix with no obvious classical version. The existence of such a classical Hamiltonian may help to answer the *prime* question but it may also lead to a real physical realization of the model. Work along this direction is in progress [40].

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## Appendix A. Wavefunctions and norms

In this appendix, we shall derive alternative expressions of the eigenfunctions of the model and compute their norm. Let us start from equation (4.12) for the eigenfunctions of the Hamiltonian (4.5),

$$\psi_E(q) = e^{-(1/2 - iE)q}\left[C_0 + \int_{-\infty}^{q} dq' e^{-iEq'}(Ba(q') - Ab(q'))\right]. \tag{A.1}$$

Replacing $a(q)$ and $b(q)$ by their Fourier transform, and using equation (5.3) one finds

$$\int_{-\infty}^{q} dq' e^{-iEq'} a(q') = \frac{\hat{a}(-E)}{2} + e^{-iqE} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{e^{iq\omega}\hat{a}(-\omega)}{\omega - E} \tag{A.2}$$

and a similar expression for the integral of $b(q)$. All the singular integrals appearing in this appendix must be understood in the Cauchy sense. Plugging the latter expressions into (A.1) yields

$$\psi_E(q) = \mathrm{e}^{-(1/2-\mathrm{i}E)q}\left[C_0 + \tfrac{1}{2}(B\hat{a}(-E) - A\hat{b}(-E)) + \mathrm{e}^{-\mathrm{i}qE}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\mathrm{e}^{\mathrm{i}q\omega}\frac{B\hat{a}(-\omega) - A\hat{b}(-\omega)}{\omega - E}\right]. \tag{A.3}$$

Using equations (4.14), (4.32) and (4.33), the first term in the rhs becomes

$$C_0 + \tfrac{1}{2}(B\hat{a}(-E) - A\hat{b}(-E)) = \tfrac{C_0+C_\infty}{2} = \mathrm{Re}\mathcal{F}(E) \tag{A.4}$$

so that $\psi(x)$ is given by

$$\psi_E(x) = \frac{\mathrm{Re}\,\mathcal{F}(E)}{x^{1/2-\mathrm{i}E}} + \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}x^{-1/2+\mathrm{i}\omega}\frac{B(E)\hat{a}(-\omega) - A(E)\hat{b}(-\omega)}{\omega - E}, \tag{A.5}$$

where $A(E)$ and $B(E)$ are given by the equations (4.32) and (4.33). The function (A.5) can also be expanded in the basis (4.3) of eigenfunctions of $H_0$, i.e.

$$|\psi_E\rangle = \int_{-\infty}^{\infty}\mathrm{d}\omega\psi_E(\omega)|\phi_\omega\rangle \tag{A.6}$$

namely

$$\psi_E(x) = \int_{-\infty}^{\infty}\mathrm{d}\omega\psi_E(\omega)\frac{x^{-1/2+\mathrm{i}\omega}}{\sqrt{2\pi}}. \tag{A.7}$$

The result is

$$\psi_E(\omega) = \sqrt{2\pi}\delta(E-\omega)\mathrm{Re}\mathcal{F}(E) + \frac{1}{\sqrt{2\pi}\mathrm{i}}\frac{B(E)\hat{a}(-\omega) - A(E)\hat{b}(-\omega)}{\omega - E}, \tag{A.8}$$

which shows that the delocalized states, i.e. $\mathcal{F}(E) \neq 0$, have to be normalized in the distributional sense, while the localized states, i.e. $\mathcal{F}(E_m) = 0$, have a norm given by

$$\langle\psi_{E_m}|\psi_{E_m}\rangle = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{|B(E_m)\hat{a}(-\omega) - A(E_m)\hat{b}(-\omega)|^2}{(\omega - E_m)^2}. \tag{A.9}$$

In the examples discussed throughout the paper the functions $\hat{a}(t)$, $\hat{b}(t)$ are phase factors, up to overall constants. Moreover, if the function $\hat{a}(t)\hat{b}(-t)$ is analytic in the upper half-plane and vanishes when $|t| \to \infty$, $\mathrm{Re}\,t > 0$, then the $S$-functions and the associated Jost function take a particular simple form if we allow for the existence of bound states,

$$S_{a,a} = S_{b,b} = 1, \qquad S_{a,b} = \hat{a}(t)\hat{b}(-t)S_{b,a} = 0 \quad\Longrightarrow\quad \mathcal{F}(t) = 2 + \hat{a}(t)\hat{b}(-t). \tag{A.10}$$

The integration constants $A$ and $B$, corresponding to a bound state, can be chosen as

$$A(E_m) = -B(E_m) = -1 \tag{A.11}$$

which differ with respect to (4.33) in an unimportant overall sign. The wavefunction (A.5) also simplifies

$$\psi_{E_m}(x) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}x^{-1/2+\mathrm{i}\omega}\frac{\hat{a}(-\omega) + \hat{b}(-\omega)}{\omega - E_m} \tag{A.12}$$

and the scalar product of two bound state wavefunctions becomes

$$\langle \psi_{E_{m_1}} | \psi_{E_{m_2}} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\mathcal{F}(\omega) + \mathcal{F}(-\omega)}{(\omega - E_{m_1})(\omega - E_{m_2})}. \tag{A.13}$$

The analiticity of the Jost function $\mathcal{F}(E)$ in the upper-half plane implies the dispersion relation

$$\mathcal{F}(E) = \mathcal{F}_\infty + \int_{-\infty}^{\infty} \frac{d\omega}{\pi i} \frac{\mathcal{F}(\omega)}{\omega - E_m}, \tag{A.14}$$

where $\mathcal{F}_\infty$ is the value of $\mathcal{F}(E)$ at $E = +i\infty$. From this equation, and the fact that $\mathcal{F}(E_{m_1}) = \mathcal{F}(E_{m_2}) = 0$, one can show that $\psi_{E_{m_1}}$ and $\psi_{E_{m_1}}$ are orthogonal. Furthermore, equation (A.14) yields also a simple expression for the norm of $\psi_{E_m}$

$$\langle \psi_{E_m} | \psi_{E_m} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\mathrm{Re}\,\mathcal{F}(\omega)}{(\omega - E_m)^2} = -\mathrm{Im}\mathcal{F}'(E_m). \tag{A.15}$$

Finally, writing $\mathcal{F}(E)$ as in equation (7.38), i.e.

$$\mathcal{F}(E) = 2(1 + \epsilon e^{2\pi i n(E)}), \tag{A.16}$$

where $n(E)$ is the number of states, up to a constant, one derives that the norm of $\psi_{E_m}$ is proportional to the density of states at $E_m$,

$$\langle \psi_{E_m} | \psi_{E_m} \rangle = 4\pi n'(E_m). \tag{A.17}$$

### *A.1. Wavefunctions associated with the smooth and exact Riemann zeros*

The Mellin transforms of the boundary wavefunctions associated with the smooth Riemann zeros were given in equation (6.10). Choosing $l_x = 1$, $l_p = 2\pi$ and $a_0 = b_0 = \sqrt{2}$ we have

$$\hat{a}(t) = \sqrt{2} e^{2i\theta(t)}, \qquad \hat{b}(t) = 1. \tag{A.18}$$

The wavefunctions (A.12) in this case become,

$$\psi_{E_m}(x) = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}\, i} x^{-1/2+i\omega} \frac{e^{-2i\theta(\omega)} + 1}{\omega - E_m}. \tag{A.19}$$

The integrals can be performed using the residue theorem obtaining

$$\frac{1}{\sqrt{2}} \psi_{E_m}(x) = \frac{H(x-1)}{x^{1/2 - iE_m}} + \frac{1}{1/4 - (iE_m/2)}\, {}_1F_2\left(\frac{1}{4} - \frac{iE_m}{2}; \frac{1}{2}, \frac{5}{4} - \frac{iE_m}{2}, -\pi^2 x^2\right), \tag{A.20}$$

where $H(x-1) = 1$, if $x > 1$ and 0, if $0 < x < 1$. One can show that $\sqrt{x}\psi_{E_m} \to 0$ as $x \to \infty$, if $1 + e^{2i\theta(E_m)} = 0$. In figure A.1, we plot the absolute values of (A.20) for those energies that correspond to the three lowest Riemann zeros. Notice that the functions are very small in the classical forbidden region $0 < x < 1$. The amplitude has a high frequency component common to the three waves plus a low frequency one that depends on the level.

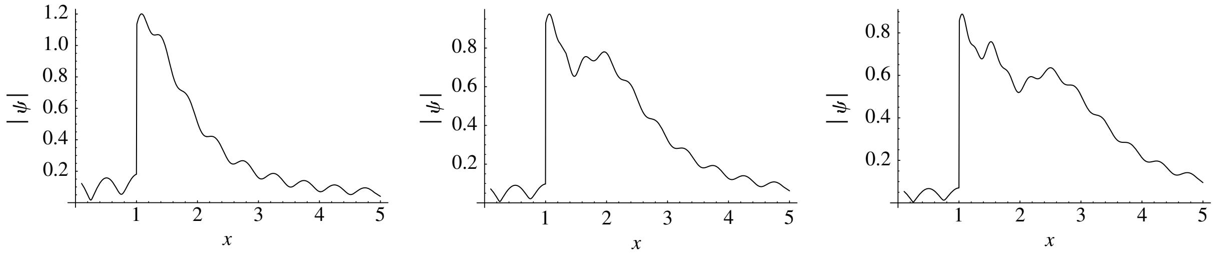


**Figure A.1.** Plot of $|\psi_{E_m}|$ for the energies $E_m = 14.5179, 20.654$ and $25.4915$, corresponding to the lowest smooth Riemann zeros (see equation (A.20)). The wavefunctions are normalized using equation (A.17).

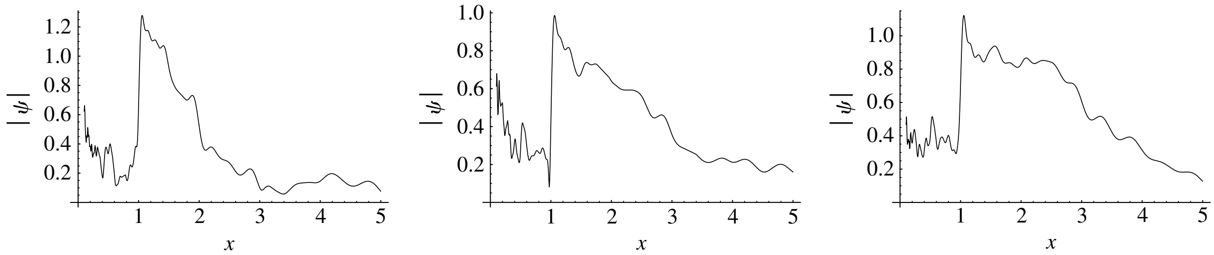


**Figure A.2.** Plot of $|\psi_{E_m}|$ for the energies Riemann zeros: 14.1347, 21.022 and 25.0109 evaluated with equation (A.21) for $\Lambda = 60$. The wavefunctions are normalized using equation (A.17).

The wavefunctions associated with the exact Riemann zeros can be computed from equation (A.12) with $\hat{a}(t)$ and $\hat{b}(t)$ given by equation (7.41). We do not have an analytic expression for this integral, however a numerical estimate can be obtained truncating (A.12) as

$$\psi_{E_m}(x) \sim \int_{E_m-\Lambda}^{E_m+\Lambda} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} x^{-1/2+\mathrm{i}\omega} \frac{\hat{a}(-\omega)+\hat{b}(-\omega)}{\omega - E_m}. \tag{A.21}$$

In figure A.2, we plot the result for the lowest Riemann zeros. The wavefunctions have some common features with those of figure A.1, but they also exhibit a random behaviour.

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