A FUNCTIONAL DETERMINANT EXPRESSION FOR THE RIEMANN XI-FUNCTION

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- ABSTRACT: We give and interpretation of the Riemann Xi-function $\xi(s)$ as the quotient of two functional determinants of an Hermitian Hamiltonian $H = H^{\dagger}$. To get the potential of this Hamiltonian we use the WKB method to approximate and evaluate the spectral Theta function $\Theta(t) = \sum_{n} \exp(-t\gamma_n^2)$ over the Riemann zeros on the critical strip $0 < \mathrm{Re}(s) < 1$. Using the WKB method we manage to get the potential inside the Hamiltonian H , also we evaluate the functional determinant $\det(H + z^2)$ by means of Zeta regularization, we discuss the similarity of our method to the method applied to get the Zeros of the Selberg Zeta function

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1. Riemann Zeta function and Selberg Zeta function

Let be a Riemann Surface with constant negative curvature and the modular group $PSL(2,R)$, Selberg [14] studied the problem of the Laplacian

$$\Delta = -y^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\Psi_n(x,y) = E_n\Psi_n(x,y) \qquad E_n = \frac{1}{4} + k_n^2 \qquad (1)$$

These momenta k_n are the non-trivial zeros of the Selberg Zeta function, which can be defined by an Euler product over the Geodesic of the surface in an analogy with the Riemann Zeta function

$$\zeta(s) = \prod_{n} \frac{1}{(1 - p_n^{-s})} \qquad Z(s) = \prod_{P}\prod_{k=0}^{\infty}\left(1 - N(P)^{-(s+k)}\right) \qquad (2)$$

Selberg also studied a Trace formula which relates the Zeros (momenta of the Laplacian Δ) on the critical line $Z\left(\frac{1}{2}+ik_n\right)=0$ and the length of the Geodesic of the Surface in the form

$$\sum_n h(k_n)=\frac{\mu(D)}{4\pi}\int_0^\infty dkkh(k)\tanh\left(\pi k\right)+\sum_{P\in p.p.o}\frac{\ln N(P)}{N(P)^{1/2}-N(P)^{1/2}}g(\ln N(P) \qquad (3)$$

Here, p.p.o means that we are taking the sum over the length of the Geodesic, $h(k)$ is a test function and $g(k)$ is the Fourier cosine transform of $h(k)$ $g(k)=\frac{1}{2\pi}\int_0^\infty dxh(x)\cos(kx)$ $\mu(D)$ is the area of the fundamental domain describing the Riemann surface . In case we had a surface with the length of the Geodesic $\ln N(P)=\ln p$ for 'p' on the second side of the equation a prime number,then the Selberg Trace is very similar to the Riemann-weil sum formula [12]

$$\sum_\gamma h(\gamma)=2h\left(\frac{i}{2}\right)-g(0)\ln\pi-2\sum_{n=1}^\infty\frac{\Lambda(n)}{\sqrt{n}}g(\ln n)+\frac{1}{2\pi}\int_{-\infty}^\infty dsh(s)\frac{\Gamma'}{\Gamma}\left(\frac{1}{4}+\frac{is}{2}\right) \quad (4)$$

This formula (4) related a sum over the imaginary part of the Riemann zeros to another sum over the primes, here $\Lambda(n)\begin{cases}\ln p & n=p^k\\ 0 & \text{otherwise}\end{cases}$ with 'k' a positive integer is the Mangoldt function, in case $\ln N(P)=\ln p$ both zeta function of Selberg and Riemann are related by $\frac{1}{Z(s)}=\prod_{n=0}^\infty\zeta\left(n+s\right)$ and their logarithmic derivative is quite similar if we set the function $\Lambda_{geodesic}(P)=\frac{\ln N(P)}{1-N(P)^{-1}}$

$$\frac{\zeta'}{\zeta}(s)=-\sum_{n=1}^\infty\Lambda(n)n^{-s} \qquad \frac{Z'}{Z}(s)=\sum_{P\in p.p.o}\Lambda_{geodesic}(P)N(P)^{-s} \qquad (5)$$

In both cases the Riemann and Selberg zeta functions obey a similar functional equation which relates the value at s and 1-s

$$Z(1-s)=\exp\left(-\frac{\mu(D)}{4\pi}\int_0^{s-1/2}vtan(\pi v)dv+c\right)Z(s) \qquad \zeta(1-s)=\mathrm{X}(s)\zeta(s) \qquad (6)$$

The constant of integration 'c' is determined by setting $s=1/2$, and $\mathrm{X}(s)=2\left(2\pi\right)^{-s}\Gamma(s)\cos\left(\frac{\pi s}{2}\right)$ for the case of the Riemann zeta function.
With the aid of the Selberg Trace formula (3) , we can evaluate the Eigenvalue staircase for the Laplacian $\Delta=-y^2\left(\partial_x^2+\partial_y^2\right)$

$$N\left(E=\frac{1}{4}+p^2\right)=\sum_{E_n\le E}1=\sum_n\frac{\mu(D)}{4\pi}\int_0^p dkkh(k)\tanh(\pi k)+\frac{1}{\pi}\arg Z\left(\frac{1}{2}+ip\right) \quad (7)$$

Here $p=\sqrt{E-\frac{1}{4}}$, we can inmediatly see that the smooth part of (7) satisfy Weyl's law in dimension 2 $N_{smooth}(E)\approx\frac{\mu(D)}{4\pi}E$, the oscillatory part of (7) satisfy Bolte's semiclassical law [4] (page 34, theorem 2.10) $\frac{1}{\pi}\arg Z\left(\frac{\lambda}{2}+i\sqrt{E}\right)$ with $\lambda=1$, the branch of the logarithm inside (7) is chosen, so $\arg Z\left(\frac{1}{2}\right)=0$ in this case the Selberg Zeta function is the dynamical zeta function of a Quantum system and the Energies are related to the zeros of $Z(s)$.

2. A functional determinant for the Riemann Xi function $\xi(s)$

From the analogies between the Riemann Zeta function and the Selberg Zeta function, we could ask ourselves if there is a Hamiltonian operator in the form

$$H\Psi_n(x)=-\frac{d^2\Psi_n(x)}{dx^2}+V(x)\Psi_n(x)=E_n\Psi_n(x) \qquad \Psi_n(0)=0=\Psi_n(\infty) \qquad E_n=\gamma_n^2 \qquad (8)$$

So for the Riemann Xi-function $\xi(s)=\frac{1}{2}s(s-1)\Gamma\left(\frac{s}{2}\right)\zeta(s)=\xi(1-s)$ we have that $\xi\left(\frac{1}{2}+i\sqrt{E_n}\right)=0 \quad \forall n\in N$, the potential is given by $V(x)\begin{cases} f(x) & x>0 \\ \infty & x\le 0\end{cases}$, at x=0 there is a infinite wall so the particle inside the well can not penetrate the region $x<0$. For the case of the Hamiltonian (8) the exact Eigenvalue staircase is [9]

$$N(E)=\sum_n H(E-E_n)=\frac{1}{\pi}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)=1+\frac{1}{\pi}\arg\zeta\left(\frac{1}{2}+i\sqrt{E}\right)+\frac{\vartheta(\sqrt{E})}{\pi} \quad (9)$$

With $H(x)\begin{cases}1 & \text{x>0}\\ 0 & \text{x<0}\end{cases}$, $\vartheta(T)=\arg\Gamma\left(\frac{1}{4}+i\frac{T}{2}\right)-\frac{T}{2}\ln\pi\approx\frac{T}{2}\ln\left(\frac{T}{2\pi e}\right)-\frac{\pi}{8}+\frac{1}{48T}+...$

As a simple example of how Quantum Mechanics can help to solve problems of finding the roots of functions , let be a particle moving inside an infinite potential well , the energy is given by $E=p^2$ and the one dimensional Schröedinger equation [7] in units $\hbar=2m=1$ ($\hbar$ is the reduced Planck's constant with value $\hbar=1.05.10^{-34}\ J.T^{-1}$)

$$H_0u_n(x)=-\frac{d^2u_n(x)}{dx^2}+V(x)u_n(x)=E_nu_n(x) \quad u_n(0)=0=u_n(\pi) \quad E_n=n^2 \qquad (10)$$

$u_n(x) = A\sin\left(\pi x\right)$, in this case the Euler's product formula for the sine function is the quotient between 2 functional determinants

$$\frac{\sin\left(\pi\sqrt{x}\right)}{\pi\sqrt{x}} = \prod_{n=1}^{\infty}\left(1-\frac{x}{E_n}\right) = \frac{\det\left(H_0 - x\right)}{\det\left(H_0\right)} \qquad H_0 = H_0^{\dagger} \qquad (11)$$

We can also compute the density of states to get the Poisson sum formula

$$\rho(E) = \sum_{n=1}^{\infty}\delta\left(E - E_n\right) = \frac{1}{2p}\left(\sum_n \delta\left(p-n\right) + \sum_n \delta\left(p-n\right)\right) = \frac{1}{2p}\sum_{n=-\infty}^{\infty} e^{2i\pi np} \qquad (11)$$

- *Zeta regularized determinant for $\xi(s)$:*

Given an Operator P with real Eigenvalues $\left\{E_n\right\}$, we can define its Zeta regularized determinant [6] in the form

$$\det\left(P + k^2\right) = \exp\left(-\frac{d}{ds}\zeta_P(s,k^2)\big|_{s=0}\right) \qquad (12)$$

Here $\zeta_P(s,k^2) = Tr\left\{(P+k^2)^{-s}\right\} = \sum_n \left(E_n + k^2\right)^{-s}$ is the Spectral Zeta function of the operator taken over all the Eigenvalues, the relationship between this spectral zeta function and the Theta function $\Theta(t) = \sum_n \exp(-tE_n)$ is given by the Mellin transform $\sum_{n=0}^{\infty}\frac{1}{\left(E_n + k^2\right)^s} = \frac{1}{\Gamma(s)}\int_0^{\infty}\frac{dt}{t}e^{-tk^2}\Theta(t)t^{s-1}$. If P is a Hamiltonian we can obtain the Theta function $\Theta(t) = \sum_n \exp(-tE_n)$ (approximately) by an integral over the Phase space [7]

$$\Theta(t) = \sum_{n=0}^{\infty}\exp\left(-tE_n\right) \approx \frac{1}{2\pi}\int_{-\infty}^{\infty}dp\int_0^{\infty}dxe^{-tp^2 - tf(x)} = \frac{1}{2\sqrt{\pi t}}\int_0^{\infty}dxe^{-tf(x)} = \Theta_{WKB}(t) \qquad (13)$$

The expression (13) depends only on the momentum and the function $f(x)$ defined in (8) to evaluate the Theta function, if we combine (13) and the definition of the Theta function for the Eigenvalues

$$\Theta(t) = \sum_{n=0}^{\infty}\exp\left(-tE_n\right) = -s\int_0^{\infty}dtN(t)e^{-st} \approx \frac{1}{2\pi}\int_{-\infty}^{\infty}dx\int_0^{\infty}dp\exp(-tp^2 - tf(x)) \qquad (14)$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}dq\int_{-\infty}^{\infty}dp\exp(-tp^2 - tf(x)) = \frac{1}{2\sqrt{\pi t}}\int_0^{\infty}dxe^{-tf(x)} = \frac{1}{2\sqrt{\pi t}}\int_0^{\infty}dre^{-tr}\frac{dV^{-1}(r)}{dr} \qquad (15)$$

From expressions (14) and (15) and setting $N(0)=0$ (after changes of variable)

$$\sqrt{s}\int_0^\infty dxN(x)e^{-sx} = \frac{1}{2\sqrt{\pi}}\int_0^\infty dxf^{-1}(x)e^{-sx} \qquad \to f^{-1}(x) = 2\sqrt{\pi}\frac{d^{1/2}}{dx^{1/2}}N(x) \qquad (16)$$

To prove (16) we have used the properties of the integral representation for the inverse Laplace transform

$$D^{\alpha}f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dsF(s)e^{st}s^{\alpha} \qquad D^{\alpha}e^{kt} = k^{\alpha}e^{kt} \quad \forall \alpha \in R \quad (17)$$

And the fact that if two Laplace transforms are equal then $L\{f(t)\} = L\{g(t)\}$ implies that $f(t)=g(t)$, for the case of the Riemann Zeros $N(E) = \frac{1}{\pi}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$ (Bolte's semiclassical law in one dimension) so $f^{-1}(x) = \frac{2}{\sqrt{\pi}}\frac{d^{1/2}}{dx^{1/2}}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$, since we want our potential inside (8) to be positive whenever we take the inverse we must choose the POSITIVE branch of the inverse in order to get $f(x)\ge 0$ on the interval $[0,\infty)$, the half derivative and the half integral for any well behaved function are given in [13]

$$\frac{d^{1/2}f(x)}{dx^{1/2}} = \frac{1}{\Gamma(1/2)}\frac{d}{dx}\int_0^x \frac{dtf(t)}{\sqrt{x-t}} \qquad \frac{d^{-1/2}f(x)}{dx^{1/2}} = \frac{1}{\Gamma(1/2)}\int_0^x dt\frac{f(t)}{\sqrt{x-t}} \quad (18)$$

We have written implicitly the potential inside (8) , if the function $f(x)$ is defined by the functional equation $f^{-1}(x) = \frac{2}{\sqrt{\pi}}\frac{d^{1/2}}{dx^{1/2}}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$, then we may evaluate the Spectral Zeta function of the Quantum system given in (8), then

$$\det\left(H+z^2\right) - det\left(H\right) = \exp\left(-\frac{d}{ds}\zeta_P(s,z^2)\big|_{s=0} + -\frac{d}{ds}\zeta_P(s,0)\big|_{s=0}\right) = \frac{\xi(z+1/2)}{\xi(1/2)} \quad (19)$$

For the potential defined by $f^{-1}(x) = \frac{2}{\sqrt{\pi}}\frac{d^{1/2}}{dx^{1/2}}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$, we can evaluate the Theta kernel uisng (15) and (16) $\Theta(t) = \sum_n \mathrm{e}^{-tE_n} = \frac{1}{2\sqrt{\pi t}}\int_0^\infty dx\frac{df^{-1}(x)}{dx}e^{-tx}$, for this potential the spectral theta function and its derivative are

$$\zeta_H(s,z^2) = \sum_{n=0}^{\infty}\frac{1}{\left(\gamma_n^2+z^2\right)^s} \qquad -\frac{d}{ds}\zeta_H(0,z^2) = \sum_{n=0}^{\infty}\ln\left(\gamma_n^2+z^2\right) \qquad \zeta\left(\frac{1}{2}+i\gamma_n\right)=0 \quad (20)$$

Taking exponentials we reach to the infinite product for the Riemann Xi-function

$$\frac{\det\left(H+z^2\right)}{\det(H)}=\frac{\prod_{n=0}^{\infty}(\gamma_n^2+z^2)}{\prod_{n=0}^{\infty}\gamma_n^2}=\prod_{n=0}^{\infty}\left(1+\frac{z^2}{E_n}\right)=\frac{\xi\left(1/2+z\right)}{\xi\left(1/2\right)} \quad (21)$$

If we choose the positive branch $f(x)\ge 0$ of the inverse $f^{-1}(x)=\frac{2}{\sqrt{\pi}}\frac{d^{1/2}}{dx^{1/2}}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$ then the potential will be always positive so the Energies of the Hamiltonian inside (8) will be all positive $E_n=\gamma_n^2\in R^+$, then all the non-trivial zeros of the Riemann Zeta function will be on the critical line $\mathrm{Re}(s)=\frac{1}{2}$, with a simple change of variable $z=s-\frac{1}{2}$ we obtain

$$\frac{\xi(s)}{\xi(0)}=\frac{\det\left(H-s(1-s)+\frac{1}{4}\right)}{\det\left(H+\frac{1}{4}\right)}=\frac{\xi(1-s)}{\xi(0)}=\prod_{\rho}\left(1-\frac{s}{\rho}\right) \quad (22)$$

Equation (22) is the Hadamard product for the Riemann Xi-function in terms of the quotient of 2 funcitonal determinants, since the expected value of the Hamiltonian is positive $\langle\psi_n\,|\,H\,|\,\psi_n\rangle\ge 0$ and Hermitian ,with $f(x)\ge 0$ then all the Energies are positive $E_n=s(1-s)\in R^+$ Riemann Hypothesis should hold.

- *Bohr-Sommerfeld quantization condition and the square of the Riemann zeros:*

The expression $f^{-1}(x)=\frac{2}{\sqrt{\pi}}\frac{d^{1/2}}{dx^{1/2}}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$ could also be obtained from the Bohr-Sommerfeld quantization conditions [7]

$$\int_C p\,dq=2\pi\left(n+\frac{1}{2}\right) \qquad 2\int_0^a dx\sqrt{E-f(x)}=p(x) \qquad E=f(a) \quad (23)$$

'a' is the classical turning point, $n=N(E)$ is the Eigenvalue staircase, the first integral inside (23) is a line integral taken over the closed orbit of the classical system, equation (23) can be understood as an integral equation for the inverse of the potential in the form

$$2\pi\left(\frac{1}{2}+n(E)\right)=2\int_0^{a=a(E)}\sqrt{E-V(x)}dx=2\int_0^E\sqrt{E-x}\,\frac{df^{-1}}{dx}=\sqrt{\pi}D_x^{-1/2}f(x) \quad (24)$$

If we take the half derivative on both sides of (24) we would get $f^{-1}(x)=2\sqrt{\pi}\frac{d^{1/2}}{dx^{1/2}}\left(\frac{1}{2}+\frac{1}{\pi}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)\right)$ in this case this result is completely equivalent to the one we got by Zeta regularization and by the WKB approximation of the Theta function $\frac{1}{2\sqrt{\pi t}}\int_0^\infty dx e^{-tf(x)}=\Theta_{WKB}(t)$.

In order to evaluate the inverse of the potential $f^{-1}(x)=\frac{2}{\sqrt{\pi}}\frac{d^{1/2}}{dx^{1/2}}\arg\xi\left(\frac{1}{2}+i\sqrt{E}\right)$ we would need to evaluate $\frac{1}{\pi}\arg\zeta\left(\frac{1}{2}+i\sqrt{E}\right)$, this can be made using the Riemann-Siegel formula [10] to evaluate the zeta function on the critical line

$$Z(k)=\zeta\left(\frac{1}{2}+ik\right)e^{i\vartheta(k)}=2\sum_{n=1}^{U(k)}\frac{\cos\left(\vartheta(k)-k\ln n\right)}{\sqrt{n}}+O\left(\frac{1}{k^{1/4}}\right)\quad k\to\infty \quad (25)$$

The functions inside (25) are $u(k)=\left[\sqrt{\frac{k}{2\pi}}\right]$, $[x]$ is the floor function and

$$\vartheta(T)=\arg\Gamma\left(\frac{1}{4}+i\frac{T}{2}\right)-\frac{T}{2}\ln\pi\approx\frac{T}{2}\ln\left(\frac{T}{2\pi e}\right)-\frac{\pi}{8}+\frac{1}{48T}+\ldots$$

- *Riemann Weyl explicit formula as the Trace $Tr\left\{\delta\left(E-f(x)\right)\right\}$:*

The next question is to compute the density of states for the Hamiltonian desfined in (8) , let be the property of the delta function $p=\sqrt{E}$ $\delta\left(E-\gamma^2\right)=\frac{\delta\left(p-\gamma\right)+\delta\left(p+\gamma\right)}{2p}$, if we use Shokhotsky's formula for the delta function $\frac{1}{-\pi}\lim_{\varepsilon\to 0}\Im m\left(\frac{1}{x-a+i\varepsilon}\right)=\delta(x-a)$, the density of states $Tr\left\{\delta\left(E-f(x)\right)\right\}$

$$-\frac{1}{\pi}\frac{d}{dE}\arg\xi\left(\frac{1}{2}+i\varepsilon+i\sqrt{E}\right)=\sum_{\gamma}\delta\left(E-\gamma^2\right)=_{reg}\frac{1}{\pi}\frac{\zeta}{\zeta}\left(\frac{1}{2}+ip\right)\frac{1}{2p}+$$
$$\frac{1}{\pi}\frac{\zeta'}{\zeta}\left(\frac{1}{2}-ip\right)\frac{1}{2p}-\frac{\ln\pi}{2\pi p}+\frac{\Gamma'}{\Gamma}\left(\frac{1}{4}+i\frac{p}{2}\right)\frac{1}{4\pi p}+\frac{\Gamma'}{\Gamma}\left(\frac{1}{4}-i\frac{p}{2}\right)\frac{1}{4\pi p}\qquad(26)$$
$$+\frac{\delta\left(p-\frac{i}{2}\right)+\pi\delta\left(p+\frac{i}{2}\right)}{2p}=\rho(E)$$

Here $\frac{1}{-\pi}\lim_{\varepsilon\to 0}\Im m\left(\frac{2}{2x\pm i+2i\varepsilon}\right)=\delta\left(x\pm\frac{i}{2}\right)$, this factor comes from the logarithmic derivative of $s(s-1)$ along the critical line $s=\frac{1}{2}+ip$, equation (26) is a distributional version of the Riemann-Weil trace formula , taking formally the logarithm of the Euler product for the Riemann Zeta function on the critical line yields to $\sum_{n=1}^{\infty}\frac{\Lambda(n)}{\sqrt{n}}e^{-ip\ln n} =_{reg} -\frac{\zeta'}{\zeta}\left(\frac{1}{2}+ip\right)$, using two test functions h(x) and g(x) $g(x)=\frac{1}{\pi}\int_{0}^{\infty}dr\cos(rx)h(r)$ we recover the oscillatory part of the Riemann-Weil trace formula $-2\sum_{n=1}^{\infty}\frac{\Lambda(n)}{\sqrt{n}}g(\ln n)$.

Unlike the model of Wu and Sprung, we have considered also the oscillatory part of the Riemann Eigenvalue Staircase $\frac{1}{\pi}\arg\zeta\left(\frac{1}{2}+i\sqrt{E}\right)$, which satisfy Bolte's semiclassical law , Wu and Sprung considered only the smooth part of teh Eigenvalue staircase in the limit $T>>1$ $\frac{T}{2\pi}\ln\left(\frac{T}{2\pi e}\right)\approx N(T)$ in order to get a Hamiltonian whose Energies are the positive imaginary part of the Riemann Zeros, their starting point is the Harmonic oscillator [15] , but unlike the normal quantum mechanical oscillator whose functional determinant gives the Gamma function $\frac{\sqrt{2\pi}}{\Gamma(s)}=\prod_{n=1}^{\infty}\left(1+\frac{s}{n}\right)$ the product taken ONLY over the positive imaginary part of the zeros (even if it converges) $\prod_{n=0}^{\infty}\left(1+\frac{s}{\gamma_n}\right)$ has no meaning, by analogy with the zeros of the Selberg Zeta function, is better to consider the case with the Energies $E_n=\gamma_n^2$, in this case the Trace of the Resolvent of the Hamiltonian $\left(E+i\varepsilon-H\right)^{-1}$ is the Riemann-Weil trace for the Riemann zeros.

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