

# A CONJECTURE ABOUT THE RIEMANN XI-FUNCTION $\xi\left(\frac{1}{2} + iz\right)$ AND FUNCTIONAL DETERMINANTS

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- **ABSTRACT:** We give a possible interpretation of the Xi-function of Riemann as the Functional determinant  $\det(E - H)$  for a certain Hamiltonian quantum operator in one dimension  $-\frac{d^2}{dx^2} + V(x)$  for a real-valued function  $V(x)$ , this potential  $V$  is related to the half-integral of the logarithmic derivative for the Riemann Xi-function, through the paper we will assume that the reduced Planck constant is defined in units where  $\hbar = 1$  and that the mass is  $2m = 1$
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## RIEMANN FUNCTION AND SPECTRAL DETERMINANTS

The Riemann Hypothesis is one of the most important open problems in mathematics, Hilbert and Polya [4] gave the conjecture that would exist an operator  $\frac{1}{2} + iL$  with

$L = L^\dagger$  so the eigenvalues of this operator would yield to the non-trivial zeros for the Riemann zeta function, for the physicists one of the best candidates would be a

Hamiltonian operator in one dimension  $-\frac{d^2}{dx^2} + V(x)$ , so when we apply the

quantization rules the Eigenvalues (energies) of this operator would appear as the solution of the spectral determinant  $\det(E - H)$ , if we define the Xi-function by

$\xi(s) = \frac{s(s-1)}{2} \Gamma\left(\frac{s}{2}\right) \zeta(s) \pi^{-s/2}$ , then RH (Riemann Hypothesis) is equivalent to the fact that the function  $\xi\left(\frac{1}{2} + iE\right)$  has REAL roots only, and then from the Hadamard

product expansion [1] for the Xi-function, then  $\frac{\xi\left(\frac{1}{2} + iE\right)}{\xi(1/2)} \approx \det(E - H)$  is an spectral (Functional) determinant of the Hamiltonian operator, if we could give an expression for the potential  $V(x)$  so the eigenvalues are the non-trivial zeros of the zeta function, then RH would follow, we will try to use the semiclassical WKB analysis [8] to obtain an approximate expression for the inverse of the potential.

Trough this paper we will use the definition of the half-derivative  $D_x^{1/2} f$  and the half integral  $D_x^{-1/2} f$ , this can be defined in terms of integrals and derivatives as

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

The case  $D_x^{3/2} f$  we can simply use the identity  $D_x^{3/2} f = \frac{d}{dx} (D_x^{1/2} f)$ , these half-integral and derivative will be used further in the paper in order to relate the inverse of the potential  $V(x)$  to the density of states  $g(E)$  that ‘counts’ the energy levels of a one dimensional  $(x,t)$  quantum system.

○ *Semiclassical evaluation of the potential  $V(x)$  :*

Unfortunately the potential  $V$  can not be exactly evaluated, a calculation of the potential can be made using the semiclassical WKB quantization of the Energy

$$\left(n(E) + \frac{1}{2}\right) 2\pi \approx 2 \int_0^{a=a(E)} \sqrt{E - V(x)} dx \rightarrow 2 \int_0^E \sqrt{E - V} \frac{dx}{dV} = \sqrt{\pi} D_x^{3/2} \left(\frac{dV^{-1}(x)}{dx}\right) \quad (2)$$

Here we have introduced the fractional integral of order  $3/2$ , for a review about fractional Calculus we recommend the text by Oldham [11], a solution to equation (2) can be obtained by applying the inverse operator  $D_x^{-1/2}$  on the left side to get

$$V^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{1/2} n(x)}{dx^{1/2}} \quad V^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{-1/2} g(x)}{dx^{-1/2}} \quad \frac{dn}{dx} = g(x) \quad (3)$$

Here  $n(E)$  or  $N(E)$  is the function that counts how many energy levels are below the energy  $E$ , and  $g(E)$  is the density of states  $g(E) = \sum_{n=0}^{\infty} \delta(E - E_n)$ , for the case of

Harmonic oscillator  $N(E) = \frac{E}{\omega}$  so using formula (2) and taking the inverse function we

recover the potential  $V(x) = \frac{\omega^2 x^2}{4}$ , which is the usual Harmonic potential for a mass

$2m = 1$  a similar calculation can be made for the infinite potential well of length 'L' with boundary conditions on  $[0, L]$  to check that our formula (3) can give coherent results

In general  $g(E)$  is difficult to calculate and we can only give semiclassical approximations to it via the Gutzwiller Trace formula [8], for the case of the Riemann Zeta function,  $N(E)$  can be defined by the equation

$$N(E) = \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + iE \right) \quad \xi(s) = \frac{s(s-1)}{2} \Gamma \left( \frac{s}{2} \right) \zeta(s) \pi^{-s/2} \quad (4)$$

So, in this case the Potential  $V(x)$  inside the one dimensional Hamiltonian operator whose energies are precisely the imaginary part of the Riemann zeros is given implicitly by the functional equation

$$V^{-1}(x) \approx \frac{1}{\sqrt{\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} + ix \right) \right) + \frac{1}{\sqrt{-\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} - ix \right) \right) \quad (5)$$

$V^{-1}(x)$  is the inverse of  $V(x)$ , taking the inverse function of formula (5) we could recover the potential at least numerically.

Using the asymptotic calculation of the smooth density of states, we could separate formula (4) into an oscillating part defined by the logarithmic derivative of the Riemann zeta function and a smooth part whose behaviour is well-known for big 'x'

$$\frac{1}{\sqrt{\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} + ix \right) \right) + \frac{1}{\sqrt{-\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} - ix \right) \right) + \frac{1}{\sqrt{\pi}} \frac{d^{1/2}}{dx^{1/2}} (x \log x - x + c) \quad (6)$$

$c = \frac{7\pi}{4}$ , Using Zeta regularization, as we did in our previous paper [6] we can expand the oscillating part of formula (6) into the divergent series

$$\frac{1}{\sqrt{\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} + ix \right) \right) + \frac{1}{\sqrt{-\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} - ix \right) \right) = 2 \sum_{n=2}^{\infty} \frac{\Lambda(n) \cos(x \log n + \pi/4)}{\sqrt{n\pi \log n}} \quad (7)$$

$\Lambda(n)$  is the Von-Mangoldt function that takes the value  $\log(p)$  if  $n = p^m$  for some positive integer 'm' and a prime p and 0 otherwise, so the last sum inside (7) involves a sum over primes and prime powers.

Then, using (3) we have found a relationship between a classical quantity, the potential

$V(x)$ , and the density of states  $g(E) = \sum_{n=0}^{\infty} \delta(E - E_n)$  of a one dimensional dynamical

system, the problem here is that  $g(E)$  can not be determined exactly unless for trivial Hamiltonians (Harmonic oscillator, potential well) the best evaluation for  $g(E)$  would

come from the Gutzwiller Trace [8] , some people believe [4] that a possible proof for the Riemann Hypothesis would follow from the quantization of an hypothetical dynamical system whose dynamical zeta function is proportional to  $\zeta\left(\frac{1}{2} + iE\right)$  to the spectral determinant of this dynamical system is  $\det(E - H) \approx e^{-iN(E)} \zeta\left(\frac{1}{2} - iE\right)$ , in this simple case the periodic orbits of the dynamical system are proportional to  $\log(p^m)$  for  $m$  positive integer and 'p' a prime number, in this case the Quantization of the Hamiltonian 'H' would yield to the imaginary part of the non-trivial zeros, these zeros then would appear to be eigenvalues (energies) of H , since H is self-adjoint /Hermitean this energies would be all REAL and all the non-trivial zeros would be of the form  $\frac{1}{2} + it \quad t \in R$ , in this case the approximate Gutzwiller Trace would be of the form

$$g(E) \approx g_{smooth}(E) + \frac{1}{\pi} \Im m \left( \frac{\partial}{\partial E} \log \zeta \left( \frac{1}{2} + iE \right) \right) \quad (8)$$

Here  $g_{smooth}(E) \approx \frac{1}{2\pi} \text{Arg} \Gamma \left( \frac{s}{2} \right) s(s-1) \pi^{-s/2}$ ,  $s = \frac{1}{2} + iE$  this contribution is well-known , for big energies E this is the main contribution to the density of states  $g(E)$  , the part involving the logarithmic derivative inside (8) is the oscillating part of the potential giving the zeros, if we combine (5) and (8) we can obtain an expression for the inverse of the potential  $V(x)$  , then solving the Hamiltonian  $H = -\frac{d^2}{dx^2} + V(x)$  with the potential given by formulae (5) and (6) we could obtain approximately the imaginary parts of the non-trivial zeros.

- *Numerical calculations of functional determinants using the Gelfand-Yaglom formula :*

In the semiclassical approach to Quantum mechanics we must calculate path integrals of the form  $\int_{\mathcal{V}} D[\phi] e^{-\langle \phi | H | \phi \rangle} \approx \frac{1}{\sqrt{\det H}}$  and hence compute a Functional determinant, one of the fastest and easiest way is the approach by Gelfand and Yaglom [2] , this technique is valid for one dimensional potential and allows you calculate the functional determinant of a certain operator 'H' without needing to compute any eigenvalue, for example if we assume Dirichlet boundary conditions on the interval [0,L]

$$\frac{\det(H + z^2)}{\det(H)} = \frac{\prod_{n=0}^{\infty} (\lambda_n - z^2)}{\prod_{n=0}^{\infty} \lambda_n} = \prod_{n=0}^{\infty} \left( 1 - \frac{z^2}{\lambda_n} \right) = \frac{\Psi^{(z)}(L)}{\Psi^{(0)}(L)} \quad (9)$$

Here the function  $\Psi^{(z)}(L)$  is the solution of the Cauchy initial value problem

$$\left(-\frac{d^2}{dx^2} + V(x) + z^2\right) \Psi^{(z)}(x) = 0 \quad \Psi^{(z)}(0) = 0 \quad \frac{d\Psi^{(z)}(0)}{dx} = 1 \quad (10)$$

For our Hilbert-Polya Hamiltonian, the imaginary part of the non-trivial zeros would appear as the solution of the eigenvalue problem  $H\phi = E_n\phi$  with the conditions

$$\phi(0) = \phi(L) = 0 \quad L \rightarrow \infty \quad V_{RH}^{-1}(x) \approx \frac{2}{\sqrt{\pi}} \Re e \left( \frac{1}{\sqrt{i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} + ix \right) \right) \right) \quad (11)$$

Since  $N(E) = \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + iE \right)$  then  $N(0) = 0$ , also the Riemann Xi-function is an

even function  $\xi(s) = \xi(1-s)$  if 's' lies on the critical line,  $s = \frac{1}{2} + iz$ , another possible

Dirichlet boundary condition is  $\phi(-L) = \phi(L) = 0$  as  $L \rightarrow \infty$ , this is equivalent to the assertion that  $\phi \in L^2(R)$ , in QM the eigenfunctions must be square-integrable

$\int_{-\infty}^{\infty} dx |\phi(x)|^2 < \infty$ , then using the Gelfand-Yaglom theorem to evaluate the spectral

determinant we find  $\frac{\det(H + z^2)}{\det(H)} = \frac{\xi \left( \frac{1}{2} + iz \right)}{\xi(1/2)} = \frac{\phi^{(z)}(L)}{\phi^{(0)}(L)}$   $L \rightarrow \infty$ , the eigenfunctions

are the solution to the problem exposed in formula (11), and they satisfy the initial value problem

$$(H + z^2)\phi^{(z)}(x) = \left(-\frac{d^2}{dx^2} + V(x) + z^2\right)\phi^{(z)}(x) = 0 \quad \phi^{(z)}(0) = 0 \quad \frac{d\phi^{(z)}(0)}{dx} = 1 \quad (12)$$

If we take the logarithm inside the Gelfand-Yaglom expression for the functional determinants [2] we can also get an expression for the spectral zeta function of

eigenvalues for integer values of 's'  $\log \frac{\det(H + z^2)}{\det(H)} = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \zeta_H(n) z^{2n}$  with

$\sum_{n=0}^{\infty} \frac{1}{\lambda_n^s} = \zeta_H(s)$ , for the case of the Riemann Xi-function, if RH is true then we should

have that the Taylor expansion of  $\log \xi \left( \frac{1}{2} + iz \right) - \log \xi \left( \frac{1}{2} \right)$  can be used to extract

information about the sums  $\sum_{n=0}^{\infty} \frac{1}{\gamma_n^k}$  involving the imaginary parts of the Riemann

zeros, in general these sums  $\sum_{n=0}^{\infty} \frac{1}{\gamma_n^k}$  can be evaluated by numerical methods so we can

compare the Taylor series of the logarithm of Xi function near  $x=0$  and these sums to check the validity (at least numerically) of Riemann Hypothesis. The condition for the functional determinant of the self-adjoint operator  $H + m^2$  to be proportional to the Xi-

function  $\xi\left(\frac{1}{2} + iz\right)$  must be imposed in order to ensure that ALL the zeros of the Riemann Zeta function are real, for example for the hyperbolic sine  $\sinh(\sqrt{x}) = \sqrt{x} \prod_{n=1}^{\infty} \left(1 + \frac{x}{n^2 \pi^2}\right)$ ,  $E_n = n^2 \pi^2$  Energies of the infinite potential well of length 1, all the roots are purely imaginary, this can be viewed as a Riemann Hypothesis for the hyperbolic sine function

○ *Why this method works ?:*

Using the semiclassical approach we have established that the inverse of potential  $V(x)$  is related to the half-derivative of the eigenvalues counting function  $N(E)$ , for the case of the infinite potential well ( $V=0$  and  $L=1$ ) the linear potential and the Harmonic oscillator, using the semiclassical WKB approach together with  $V^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}}$

$$\text{Harmonic oscillator } V = \frac{(\omega x)^2}{4} \quad N(E) = \frac{E}{\omega} \quad V^{-1}(x) = \frac{2\sqrt{E}}{\omega} \quad (13)$$

$$\text{Linear potential } V = k|x| \quad N(E) = \frac{2E^{3/2}}{3\pi k} \quad V^{-1}(x) = \frac{x}{k} \quad (14)$$

$$\text{Infinite potential well } V = 0 \quad N(E) = \frac{\sqrt{E}}{\pi} \quad V^{-1}(x) = 1 \quad (15)$$

In all cases and for simplicity we have used the notation  $\hbar = 2m = 1 = L$ , here 'L' is the length of the well inside (15), (13) and (14) are correct results that one can obtain using the exact Quantum theory and (15) gives 1 instead of the expected result  $V = 0$ , in order to calculate the fractional derivatives for powers of E we have used the identity

$$\frac{d^{1/2} E^k}{dE^{1/2}} = \frac{\Gamma(k+1)}{\Gamma(k+1/2)} E^{k-1/2} \quad [11], \text{ a similar formal result can be applied to Bohr's atomic}$$

$$\text{model for the quantization of Energies inside Hydrogen atom } E = -\frac{13.6}{n^2}.$$

For the general case of the potentials  $V = C|x|^m$  with m being a Natural number our formula,  $V^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}}$  predicts that the approximate number of energy levels

$$\text{below a certain Energy E will be (approximately) } N(E) = \frac{1}{\sqrt{4\pi}} \frac{\Gamma\left(\frac{1}{m} + 1\right)}{\Gamma\left(\frac{1}{m} + \frac{3}{2}\right)} E^{\frac{1}{m} + \frac{1}{2}}, \text{ see}$$

[11] for the definition of the half-integral for powers of 'x'. It was prof. Mussardo [10] who gave a similar interpretation to our formula  $V^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}}$  in order to calculate the Quantum potential for prime numbers, he reached to the conclusion that

the inverse of the potential inside the Quantum Hamiltonian  $-\frac{d^2}{dx^2} + V(x) = H$  giving the prime numbers as Eigenvalues/Energies of H , should satisfy the equation

$V^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{1/2}\pi(x)}{dx^{1/2}}$  , here  $\pi(x) = \sum_{p \leq x} 1$  is the Prime counting function that tells us how many primes are below a given real number x , there is no EXACT formula for  $\pi(x) = \sum_{p \leq x} 1$  so Mussardo used the approximate expression for the derivative given by

the Ramanujan formula  $\frac{d\pi(x)}{dx} \approx \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{x^{1/n}}{\log x} \right)$  [10] , where  $\mu(n)$  is the

Mobius function , a number-theoretical function that may take the values -1,0, 1 ( see Apostol's book [1] for further information ).

A formal justification of why the density of states is related to the imaginary part of the logarithmic derivative of  $\xi \left( \frac{1}{2} + iz \right)$  can be given as the following, let us suppose that the Xi-function has only real roots , then in the sense of distribution we can write

$$\frac{\xi'}{\xi} \left( \frac{1}{2} + iz \right) = \sum_{n=-\infty}^{\infty} \frac{a_n}{x + i\varepsilon - \gamma_n} \quad a_n = \text{Re} s \left( z = \gamma_n, \frac{\xi'}{\xi} \right) \quad (16)$$

Here,  $\varepsilon \rightarrow 0$  is a small quantity to avoid the poles of (16) at the Riemann Non-trivial zeroes  $\{\gamma_n\}$  ,taking the imaginary part inside the distributional Sokhotsky's formula

$$\frac{1}{x - a + i\varepsilon} = -i\pi\delta(x - a) + P \left( \frac{1}{x - a} \right) \text{ one gets the density of states}$$

$$g(E) = \frac{1}{\pi} \Im m \partial_E \log \xi \left( \frac{1}{2} + iE \right) = - \sum_{n=-\infty}^{\infty} \delta(E - \gamma_n) \quad (17)$$

Integration with respect to E will give the known equation  $N(E) = \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + iE \right)$  , a

similar expression can be obtained via the 'argument principle' of complex integration

$$N(E) = \frac{1}{2\pi i} \int_{D(E)} \frac{\xi'}{\xi} (z) dz \text{ , with } D \text{ a contour that includes all the non-trivial zeros below}$$

a given quantity E , the density of states can be used to calculate sums over the Riemann zeta function (nontrivial) zeros, for example let be the identities

$$\sum_{\gamma} f(\gamma) = -\frac{1}{\pi} \int_0^{\infty} ds f'(s) \text{Arg} \xi \left( \frac{1}{2} + is \right) \quad \frac{\zeta'}{\zeta} \left( \frac{1}{2} + iz \right) = \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} e^{is \log n} \quad (18)$$

Combining these both [6] we can prove the Riemann-Weyl summation formula

$$\sum_{\gamma} f(\gamma) = 2f \left( \frac{i}{2} \right) - g(0) \log \pi - 2 \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} g(\log n) + \frac{1}{2\pi} \int_{-\infty}^{\infty} ds f'(s) \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} + \frac{is}{2} \right) \quad (19)$$

With  $f(x) = f(-x)$  and  $g(x) = g(-x)$  and  $g(y) = \frac{1}{\pi} \int_0^{\infty} dx \cos(yx) f(x)$

## CONCLUSIONS AND FINAL REMARK

Using the semiclassical analysis and the WKB quantization of energies, we have managed to prove that for one dimensional systems the inverse of the potential inside

the Hamiltonian  $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$  ( for simplicity through this paper we have used

the notation  $\hbar = 1 = 2m$  to simplify calculation) is related to the half-derivative of the energy counting function  $N(E)$  or the half-integral of the density of states

$g(E) = \sum_{n=0}^{\infty} \delta(E - E_n)$  in the (approximate) form  $V^{-1}(x) \approx \sqrt{\frac{2\pi\hbar^2}{m} \frac{d^{-1/2}g(x)}{dx^{-1/2}}}$ . From the

definition of the counting function  $N(T)$  for the nontrivial zeros of the Riemann Zeta

function lying on the critical strip  $N(E) = \frac{1}{\pi} \text{Arg} \xi\left(\frac{1}{2} + iE\right)$  and using our formula (2)

with  $2m=1$  we have obtained the semiclassical approximation for the inverse of the potential  $V(x)$  (4) and have given some Numerical test that could be done in order to check that our definition for the inverse of the potential  $V^{-1}(x)$  can be used to obtain a Hilbert-Polya differential operator whose eigenvalues (Energies) are precisely the imaginary part of the non-trivial zeros of the Riemann Zeta function, in case our formula is correct and (4) is the potential of a Hilbert-Polya operator satisfying Riemann Hypothesis then imposing Dirichlet boundary conditions  $[0, L]$  with  $L \rightarrow \infty$  then the

Gelfand-Yaglom formula should give  $\frac{\xi\left(\frac{1}{2} + iz\right)}{\xi(1/2)} = \frac{\det(H + z^2)}{\det(H)} = \frac{\phi^{(z)}(L)}{\phi^{(0)}(L)}$   $L \rightarrow \infty$  so

the functional determinant of  $H = -\frac{d^2}{dx^2} + V(x)$  is proportional to the Riemann Xi-

function , this potential  $V(x)$  is given implicitly in (5) and (6) . A possible better

improvement of our formula (3) would be to write down  $V^{-1}(x) \approx A \frac{d^{1/2}n(x)}{dx^{1/2}}$  for some

constant 'A' to be fixed in order to obtain (if possible) the correct energies of our Hamiltonian at least when  $n \rightarrow \infty$   $E_n$  , for simplicity since the spatial term

(derivative) inside Schröedinger equation takes the form  $\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$  we chose

$\hbar = 2m = 1$  to simplify calculations.

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