

# A HAMILTONIAN OPERATOR WHOSE ZEROS ARE THE ROOTS OF THE RIEMANN XI-FUNCTION $\xi\left(\frac{1}{2}+i\sqrt{z}\right)$

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ullet ABSTRACT: We give a possible interpretation of the Xi-function of Riemann as the Functional determinant  $\det \left( E-H \right)$  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 exists 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

 $\xi\left(s\right) = \frac{s(s-1)}{2}\Gamma\left(\frac{s}{2}\right)\zeta(s)\pi^{-s/2}$ , 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 
$$\frac{\xi\left(\frac{1}{2}+iE\right)}{\xi(1/2)} = \det(E-H)$$
 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

$$\frac{d^{1/2}f(x)}{dx^{1/2}} = \frac{1}{\Gamma(1/2)} \frac{d}{dx} \int_{0}^{x} \frac{dt f(t)}{\sqrt{x-t}} \qquad \frac{d^{-1/2}f(x)}{dx^{1/2}} = \frac{1}{\Gamma(1/2)} \int_{0}^{x} dt \frac{f(t)}{\sqrt{x-t}}$$
(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.

 $\circ$  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

$$2\pi n(E) = 2\int_{0}^{a=a(E)} \sqrt{E - V(x)} dx \to 2\int_{0}^{E} \sqrt{E - V} \frac{dx}{dV} = \sqrt{\pi} D_{x}^{-3/2} \left(\frac{dV^{-1}(x)}{dx}\right)$$
(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] for a good introduction to fractional calculus, a solution to equation (2) can be obtained by applying the inverse operator  $D_x^{1/2}$  on the left side to get

$$V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}} \qquad V^{-1}(x) = 2\sqrt{\pi} \frac{d^{-1/2}g(x)}{dx^{-1/2}} \qquad \frac{dn}{dx} = g(x)$$
 (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  $[0, \infty)$  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

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

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

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

 $V_{RH}^{-1}(x)$  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'

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

$$\frac{1}{\sqrt{\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\zeta'}{\zeta} \left( \frac{1}{2} + ix \right) \right) + \frac{1}{\sqrt{-\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\zeta'}{\zeta} \left( \frac{1}{2} - ix \right) \right) = 2 \sum_{n=2}^{\infty} \frac{\Lambda(n) \cos(x \log n + \pi/4)}{\sqrt{n\pi \log n}}$$
(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  $\det\left(E-H\right)=e^{-iN(E)}\zeta\left(\frac{1}{2}-iE\right)$ , in this simple case the periodic orbits of the dynamical system are proportional to  $\log\left(p^m\right)$  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  $\frac{1}{2}+it$   $t\in R$ , in this case the approximate Gutzwiller Trace would be of the form

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

Here  $g_{smooth}(E) \approx \frac{1}{2\pi} \log(E)$ ,  $s = \frac{1}{2} + iE$  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 nontrivial zeros. If we used the EKB quantization condition (Quantum chaos)  $\int_C pdq = n + \frac{\mu}{4}$ , then formula (3) becomes  $V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2}}{dx^{1/2}} \left( n(E) + \frac{\mu}{4} \right)$ , so inside the inverse of the potential an extra term of the form  $\frac{\mu}{\sqrt{4\pi}}$ , here  $\mu$  is a extra

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

geometrical constant that appears in the semiclassical EKB quantization.

assume Dirichlet boundary conditions on the interval  $[0,\infty)$ 

In the semiclassical approach to Quantum mechanics we must calculate path integrals of the form  $\int_V D[\phi] e^{-\langle \phi|H|\phi\rangle} = \frac{1}{\sqrt{\det H}}$  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

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

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

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

For our Hilbert-Polya Hamiltonian, the imaginary part of the non-trivial zeros would appear as the solution of the eigenvalue problem  $H\phi = E_n\phi$  so  $E_n = \gamma_n$  (imaginary part of the Riemann zeros ) with the boundary condition

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

Since  $N(E)=\frac{1}{\pi}Arg\xi\left(\frac{1}{2}+iE\right)$  then N(0)=0, also the Riemann Xi-function is an even function because  $\xi(s)=\xi(1-s)$ ,  $s=\frac{1}{2}+iz$ , another possible Dirichlet boundary conditions are  $\phi(-L)=\phi(L)=0$  as  $L\to\infty$ , this is equivalent to the assertion that  $\phi\in L^2(R)$ , in QM the eigenfunctions must be square-integrable  $\int\limits_{-\infty}^{\infty}dx\left|\phi(x)\right|^2<\infty$ , then we could use the Gelfand-Yaglom theorem to evaluate the spectral determinants so for our Hamiltonian operator H we find the formula

$$\frac{\det(H-z)}{\det(H)} \cdot \frac{\det(H+z)}{\det(H)} = \frac{\xi\left(\frac{1}{2} + iz\right)}{\xi\left(1/2\right)} = \frac{\phi^{(z)}(L)}{\phi^{(0)}(L)} \cdot \frac{\phi^{(-z)}(L)}{\phi^{(0)}(L)} \cdot L \to \infty \quad (12)$$

the functions  $\phi^{(\pm z)}(x)$  defined in (12) satisfy the initial value problem

$$(H \pm z)\phi^{(\pm z)}(x) = \left(-\frac{d^2}{dx^2} + V(x) \pm z\right)\phi^{(\pm z)}(x) = 0 \qquad \phi^{(\pm z)}(0) = 0 \qquad \frac{d\phi^{(\pm z)}(0)}{dx} = 1$$
 (13)

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'

$$\log\frac{\det\left(H-z\right)}{\det(H)} + \log\frac{\det\left(H+z\right)}{\det(H)} = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\zeta_H(n)z^{2n} \text{ with } \sum_{n=0}^{\infty}\frac{1}{\lambda_n^s} = \zeta_H(s) \text{ , for the case of the Riemann Xi-function , if RH is true then we should have that the Taylor expansion of } \log\xi\left(\frac{1}{2}+z\right) - \log\xi\left(\frac{1}{2}\right) \text{ can be used to extract information about the}$$

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  $(H+\lim)(H-ilm)$  to be proportional to the function  $\xi\left(\frac{1}{2}+x\right)=\prod_{n=1}^{\infty}\left(1+\frac{x^2}{\gamma_n^2}\right)$  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 , another example is the cosine function  $d(x)=\cos\left(\frac{\pi x}{\omega}\right)$ , whose roots are precisely the energies of the Quantum harmonic oscillator  $E_n=\left(n+\frac{1}{2}\right)\omega$  , and the density of states is defined by the Poisson summation formula  $\sum_{n=0}^{\infty}\delta\left(x-n\omega-\frac{\omega}{2}\right)=g(x)=\sum_{n=0}^{\infty}(-1)^ne^{\frac{2\pi inx}{\omega}}$ 

## GENERALIZATION TO A HAMILTONIAN WHOSE ENERGIES ARE THE SQUARE OF THE IMAGINARY PART OF THE RIEMANN NON-TRIVIAL ZEROS

We can generalize these results to the case of a Hamiltonian whose Energies are just the square of the imaginary part of Riemann zeros  $E_n = \gamma_n^2$ , in this case the Energy counting function is given by  $N(E) = \frac{1}{\pi} Arg \xi \left( \frac{1}{2} + i \sqrt{E} \right)$  (since now we are counting squares of the Riemann zeros), using the same reasoning we did in (5) to get the inverse of the potential, for this Hamiltonian operator  $-\partial_x^2 + V_2(x) = H_2$   $\partial_x^2 = \frac{d^2}{dx^2}$  we get

$$V^{-1}_{2}(x) \approx \frac{1}{\sqrt{4\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} + i\sqrt{x} \right) \frac{1}{\sqrt{x}} \right) + \frac{1}{\sqrt{-4\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\xi'}{\xi} \left( \frac{1}{2} - i\sqrt{x} \right) \frac{1}{\sqrt{x}} \right)$$
(14)

In this case the functional determinant of this Hamiltonian should be

$$\frac{\det(H_2 - z)}{\det(H_2)} = \frac{\prod_{n=0}^{\infty} (E_n - z)}{\prod_{n=0}^{\infty} E_n} = \prod_{n=0}^{\infty} \left(1 - \frac{z}{\gamma_n^2}\right) = \frac{\xi(1/2 + i\sqrt{z})}{\xi(1/2)} \quad z > 0 \quad (15)$$

In this case the Hamiltonian would be bounded so  $\langle H_2 \rangle \ge \gamma_0^2 = 199.750490$ .. since we are dealing with 1-D potential the functional determinant inside (15) can be calculated using the Gelfand-Yaglom Theorem and it will be equal to

$$\frac{\det(H_2 - z)}{\det(H_2)} = \frac{\Psi^{(z)}(L)}{\Psi^{(z)}(0)} \text{ with } \left(-\partial_x^2 + V_2(x) - z\right) \Psi^{(z)}(x) = 0 \quad (16)$$

Plus the initial value conditions  $\Psi^{(z)}(0) = 0$  and  $\frac{d\Psi^{(z)}(0)}{dr} = 1$ .

As a toy model of this method, let be the Sturm-Liouville problem  $-\frac{d^2y(x)}{dx^2} = E_n y(x)$  with boundary conditions y(0) = y(1) = 0, this problem can be easily solved to prove that the Energies and the functional determinant are the following

$$E_n = n^2 \pi^2$$
  $n = 1, 2, 3, ...$   $\frac{\sin(\sqrt{x})}{\sqrt{x}} = \prod_{n=1}^{\infty} \left(1 - \frac{x}{n^2 \pi^2}\right)$  (17)

If we use the expansion of the cotangent plus the Sokhotsky's formula

$$\frac{1}{x+i\varepsilon} = -i\pi\delta(x) + P\left(\frac{1}{x}\right) \qquad \frac{\cot(x)}{2x} - \frac{1}{2x^2} = \sum_{n=1}^{\infty} \frac{1}{x^2 - n^2\pi^2 + i\varepsilon}$$
(18)

The factor  $i\varepsilon$  is introduced in order (18) to be regular at the points  $n^2\pi^2$  for any positive integer 'n' bigger than 1 if we take the imaginary part inside (18) we have that

$$\frac{1}{\pi} \Im mg \left( \frac{\cot(x)}{2x} - \frac{1}{2x^2} \right) = -\sum_{n=1}^{\infty} \delta(x^2 - n^2 \pi^2) \text{ making the substitution } x \to \sqrt{E} \text{ the last}$$

term is just the derivative of N(E) in the case of the Infinite potential well so in formal sense (theory of distributions) one expects that the number of eigenvalues of the

problem 
$$-\frac{d^2y(x)}{dx^2} = E_n y(x)$$
 is given by the following formal formula

$$N(E) = \frac{1}{\pi} Arg \left( \frac{\sin \sqrt{E}}{\sqrt{E}} \right)$$
. Here 'reg' means that we should replace the factor

 $(x-a)^{-1}$  (singular at the point a) by the distribution  $(x+i\varepsilon-a)^{-1}$  with  $\varepsilon\to 0$ , hence one could hope that the same would be valid for the Riemann Xi-function, so if we repeat our same argument for the Riemann Hypothesis we find

$$N(E) = \frac{1}{\pi} Arg \xi \left( \frac{1}{2} + i\sqrt{E} \right)_{reg} \qquad \frac{\xi'}{\xi} \left( \frac{1}{2} + i\sqrt{x} \right) \frac{1}{2\sqrt{x}}_{reg} = \sum_{n=0}^{\infty} \frac{a_n}{x + i\varepsilon - \gamma_n^2} \quad \left\{ a_n \right\} \in R \quad (19)$$

Another more complicate example is the differential equation  $x\frac{d^2y}{dx^2}+\frac{dy}{dx}+\lambda_ny=0$  with the boundary conditions y(1)=0 and with a solution bounded as  $x\to 0$ , the equation for the Eigenvalues is given by the square of zeros of the Bessel function  $J_0(\sqrt{\lambda_n})=0$ , the Eigenvalue counting function is then  $N(E)=\frac{1}{\pi}Arg\left(J_0(\sqrt{E})\right)_{reg}$ , this is another example of how the Eigenvalues of certain self-adjoint operator are related to the roots of a function that has a product expansion over its zeros in the form  $J_0(\sqrt{x})=J_0(0)\prod_{n=0}^{\infty}\left(1-\frac{x}{\alpha_n^2}\right)$ , in case Riemann Hypothesis is true (and the self-adjoint operator is a Hamiltonian whose potential is given in (14)) the Gelfand-Yaglom theorem used to compute the quotient of two functional determinants, could be used to give a representation of the Riemann Xi-function

$$\frac{\det\left(-\partial_{x}^{2}+V_{2}-z\right)}{\det(-\partial_{x}^{2}+V_{0}-z)} = \frac{\Psi^{(z)}(L)}{\Psi_{free}^{(z)}(L)} = \frac{\xi\left(\frac{1}{2}+i\sqrt{z}\right)}{\xi\left(1/2\right)} \qquad L \to \infty , \ V_{0} = 0 \qquad (20)$$

With the initial conditions,  $\Psi^{(z)}(0) = 0 = \Psi_{free}^{(z)}(0)$  and  $\frac{d\Psi^{(z)}(0)}{dx} = 1 = \frac{d\Psi_{free}^{(z)}(0)}{dx}$ , the Riemann Xi-function can be expressed as the quotient of 2 Functional determinants, from (20) we get the usual Semiclassical quantization condition namely  $\det\left(-\partial_x^2 + V_2 - E\right) = 0$ , the roots of the functional determinant will be the Eigenvalues of the Hamiltonian operator  $E_n = \gamma_n^2 = E$ , the boundary conditions chosen for this Hamiltonian will be the following  $\Psi(0) = 0 = \Psi(\infty)$  in order to evaluate the determinant (20), as always the functions  $\Psi^{(z)}(x)$ ,  $\Psi_{free}^{(z)}(x)$  are evaluated by solving the initial value problem  $\left(-\partial_x^2 + V_j - z\right)\Psi_j^{(z)}(x) = 0$  with  $\Psi_j^{(z)}(0) = 0$   $\frac{d\Psi_j^{(z)}(0)}{dx} = 1$ . In order to solve this last equation one could use the WKB semiclassical approximation so  $\Psi_j^{(z)}(x)$  can be approximated by

$$\Psi_{j}^{(z)}(x) \approx \left(z - V_{2}(x)\right)^{-1/4} \left\{ C_{+} \exp\left(i \int_{0}^{x} \sqrt{z - V_{2}(t)} dt\right) + C_{-} \exp\left(-i \int_{0}^{x} \sqrt{z - V_{2}(t)} dt\right) \right\}$$
(21)

The constants  $C_{\pm}$  are obtained from the initial value conditions for the wavefunction, they satisfy the equation  $C_{+} + C_{-} = 0$  since  $\Psi_{j}^{(z)}(0) = 0$ 

Also if we add a term  $\frac{1}{4}$  to the potential  $V_2(x)$  inside (14) then the eigenvalues wouls be  $|s|^2 = \frac{1}{4} + \gamma_n^2$  the square of the modulus of the Riemann Zeros. The condition for the determinant to be proportional to  $\xi\left(\frac{1}{2} + i\sqrt{E}\right)$  is a necessary and sufficient condition to

prove RH, due to the self-adjointness of  $H_2 = H_2^{\dagger}$ , the condition for the potential  $V_2^{-1}(x) \approx \frac{2}{\sqrt{\pi}} \frac{d^{1/2}}{dx^{1/2}} Arg \xi \left(\frac{1}{2} + i\sqrt{x}\right)$  itself is not enough since there could still be some imaginary zeros of the Riemann Xi-function that would not appear inside the spectrum of the Hamiltonian, note that this is similar what it happened with the Quantum mechanical model for the zeros of the sine and Bessel functions  $\sin\left(\sqrt{x}\right)$ ,  $J_0(\sqrt{x})$ . As we have pointed out before  $Argf(x)_{reg} = Argf(x+i\varepsilon)$ , so  $\Im m\left\{\frac{f'(x+i\varepsilon)}{f(x+i\varepsilon)}\right\} = -\frac{1}{\pi} \frac{dn}{dx}$  is only nonzero for the values  $f(x_i) = 0$ , n(x) here 'counts' the zeros of f(x).

# NUMERICAL CALCULATIONS AND THE LINK BETWEEN THE RIEMANN-WEYL FORMULA FOR PRIMES AND THE DENSITY OF STATES OF OUR HAMILTONIAN $\rm H_2$

In this section we will explain why this method works, also we will compare our trace with the explicit formula of Riemann and Weyl relating a sum involving primes to another sum involving the imaginary part of the zeros.

#### • Why this method works?:

Using the semiclassical approach we have stablished 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  $V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}}$ 

Harmonic oscillator 
$$V = \frac{(\omega x)^2}{4}$$
  $N(E) = \frac{E}{\omega}$   $V^{-1}(x) = \frac{2\sqrt{E}}{\omega}$  (22)

Linear potential 
$$V = kx$$
  $N(E) = \frac{2E^{3/2}}{3\pi k}$   $V^{-1}(x) = \frac{x}{k}$  (23)

Infinite potential well 
$$V = 0$$
  $N(E) = \frac{\sqrt{E}}{\pi}$   $V^{-1}(x) = 1$  (24)

In all cases and for simplicity we have used the notation  $\hbar = 2m = 1 = L$ , here 'L' is the length of the well inside (22), (23) and (24) are correct results that one can obtain using the exact Quantum theory, (24) 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

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

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

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

below a certain Energy E will be (approximately)  $N(E) = \frac{1}{\sqrt{4\pi}} \frac{\Gamma\left(\frac{1}{m}+1\right)}{\Gamma\left(\frac{1}{m}+\frac{3}{2}\right)} E^{\frac{1}{m}+\frac{1}{2}}$ , 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  $V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}}$  in order to calculate the Quantum potential for prime numbers, he reached to the conclussion 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  $V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2}\pi(x)}{dx^{1/2}}$ , here  $\pi(x) = \sum_{p \le x} 1$  is the Prime counting function that tells us how many primes are below a given real number x , there is no EXACT formula for  $\pi(x) = \sum_{p \le x} 1$  so Mussardo used the approximate expression for the derivative given by

the Ramanujan formula  $\frac{d\pi(x)}{dx} = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \frac{d^{-1/2}}{dx^{-1/2}} \left(\frac{x^{1/n}}{\log x}\right)$  [10], where  $\mu(n)$  is the Mobius function, a number-theoretical function that may take the values -1,0,1 (see Apostol [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

$$\frac{\xi'}{\xi} \left( \frac{1}{2} + i\sqrt{z} \right) = \sum_{n=0}^{\infty} \frac{a_n}{z + i\varepsilon - \gamma_n^2} \qquad a_n = \operatorname{Re} s \left( z = \gamma_n, \frac{\xi'}{\xi} \right)$$
 (25)

Here,  $\varepsilon \to 0$  is an 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

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

$$g(E) = \frac{1}{\pi} \Im m \partial_E \log \xi \left( \frac{1}{2} + iE \right) = -\sum_{n = -\infty}^{\infty} \delta(E - \gamma_n)$$
 (26)

Integration with respect to E will give the known equation  $N(E) = \frac{1}{\pi} Arg \xi \left( \frac{1}{2} + iE \right)$ , a similar expression can be obtained via the 'argument principle' of complex integration

 $N(E) = \frac{1}{2\pi i} \int_{D(E)} \frac{\xi'}{\xi}(z) dz$ , with D 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

$$\sum_{\gamma} f(\gamma) = -\frac{1}{\pi} \int_{0}^{\infty} ds f'(s) Arg \xi\left(\frac{1}{2} + is\right) \qquad -\frac{\zeta'}{\zeta} \left(\frac{1}{2} + iz\right) = \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} e^{is\log n}$$
 (27)

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

$$\sum_{\gamma} f(\gamma) = 2f\left(\frac{i}{2}\right) - g(0)\log \pi - 2\sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} g(\log n) + \frac{1}{2\pi} \int_{-\infty}^{\infty} ds f(s) \frac{\Gamma'}{\Gamma} \left(\frac{1}{4} + \frac{is}{2}\right)$$
(28)

With 
$$f(x) = f(-x)$$
 and  $g(x) = g(-x)$  and  $g(y) = \frac{1}{\pi} \int_{0}^{\infty} dx \cos(yx) f(x)$ , if we are

allowed to put  $f = \cos(ax)$  into (20), then the Riemann-Weyl formula can be regarded as an exact Gutzwiller trace for a dynamical system with Hamilton equations

$$2p = \dot{x} \qquad \dot{p} = -\frac{\partial V}{\partial x} \qquad n(E) = \frac{1}{\pi} Arg \xi \left(\frac{1}{2} + iE\right) \qquad V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2}n(x)}{dx^{1/2}} \quad (29)$$

Then the Gutzwiller trace for this dynamical one dimensional system (x,t) is  $g(E) = g_{smooth}(E) + \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} \cos(E \log n) \text{ , for big E the smooth part can be}$  approximated by  $g_{smooth}(E) \approx \frac{\log E}{2\pi} \text{ . The sum involving the Mangold function } \Lambda(n)$  is divergent, however it can be regularized in order to give the real part of the logarithmic derivative of Riemann Zeta  $-\frac{\zeta'}{\zeta} \left(\frac{1}{2} + iE\right)$ 

• Numerical solution of Schröedinguer equation:

In order to solve our operator  $-\frac{d^2}{dx^2} + V_2(x) = H$  with boundary conditions y(0) = y(L) = 0  $L = 10^6$  we need to calculate the potential  $V_2(x)$ , first since  $V_2^{-1}(x) \approx \frac{2}{\sqrt{\pi}} \frac{d^{1/2}}{dx^{1/2}} Arg \xi \left(\frac{1}{2} + i\sqrt{x}\right)$  we may use the Grunwald-Letnikov definition of the half-derivative to write the inverse of the potential in the form

$$V_2^{-1}(x) \approx \frac{2}{\sqrt{\pi\varepsilon}} \sum_{m=0}^{\infty} {1/2 \choose m} (-1)^m \operatorname{Arg} \xi \left( \frac{1}{2} + i \sqrt{x + \left(\frac{1}{2} - m\right)\varepsilon} \right)$$
 (30)

Here ' $\varepsilon$ ' is an small step used to define the fractional derivative and  $\binom{n}{m} = \frac{\Gamma(n+1)}{\Gamma(m+1)\Gamma(n-m+1)}$  are the binomial coefficients, giving values of 'x' inside (30) we can compute the inverse of the potential  $V_2(x)$ , in order to get  $V_2(x)$ , we simply reflect every point  $(x_j, V_2^{-1}(x_j))$  obtained in formula (30) across the line y = x to get the numerical values for the potential  $V_2(x_j)$ , we have solved numerically the Schröedinguer equation for  $V_2(x)$  using this method to obtain

n	0	1	2	3	4
Roots <sup>2</sup>	199.7897	441.9244	625.5401	925.6684	1084.7142
Eigenvalues	198.8351	441.9101	625.5950	925.6398	1084.6789

The final step is to solve the initial value problem  $\left(-\partial_x^2 + f(x) - z\right)y_z(x) = 0$  with  $y_z(0) = 0$  and  $\frac{dy_z(0)}{dx} = 1$  for  $f(x) = V_2(x)$  and for f(x) = 0 (free particle) in order to obtain the functional determinant  $\xi\left(\frac{1}{2} + i\sqrt{z}\right) = \xi\left(\frac{1}{2}\right) \prod_{n=0}^{\infty} \left(1 - \frac{z}{\gamma_n^2}\right) = \frac{y_{(z)}(L)}{y_{(z)\,free}(L)}$   $L \to \infty$ 

#### o Corrections to the Wu-Sprung potential:

We can split our inverse potential into 2 terms, a first term is proportional to the real part of the Half integral of  $\frac{\zeta'}{\zeta} \left( \frac{1}{2} + i \sqrt{s} \right)$ , and an smooth part that was known to Wu and Sprung [14], that used the approximation  $N(T) \approx \frac{T}{2\pi} \log \frac{T}{2\pi} - \frac{T}{2\pi}$  for big 'T'

$$V^{-1}(x) = \frac{1}{\sqrt{\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\zeta'}{\zeta} \left( \frac{1}{2} + ix \right) \right) + \frac{1}{\sqrt{-\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\zeta'}{\zeta} \left( \frac{1}{2} - ix \right) \right) - \frac{\sqrt{x}}{\pi^{3/2}} \log \pi + \frac{1}{\sqrt{2\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} + \frac{ix}{2} \right) \right) + \frac{1}{\sqrt{-2\pi i}} \frac{d^{-1/2}}{dx^{-1/2}} \left( \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} - \frac{ix}{2} \right) \right)$$
(31)

Here  $\Lambda(n)$  stands for the Von Mangoldt function, that takes the value  $\log p$  iff  $n = p^k$   $k \in N$  and 0 otherwise. The first part is just the oscillating contribution to the potential produced by the distribution of the prime numbers, and it is equal to the zeta-regularized value of the sum  $\sum_{n=1}^{\infty} \frac{\Lambda(n) \cos \left(s \log n + \pi/4\right)}{\sqrt{n \log n}}$ , the idea is that the potential

V(x) must be compatible with the semiclassical approximation of Quantum mechanics, but also if the imaginary part of the zeros are the Eigenvalues of a certain operator, it must also obey the Rieman-Weyl trace formula relating primes and Riemann Zeta zeros

$$\sum_{\gamma} h(\gamma) = 2h\left(\frac{i}{2}\right) - 2\sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} g(\log n) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dr h(r) \frac{\Gamma'}{\Gamma} \left(\frac{1}{4} + \frac{ir}{2}\right) - g(0) \log \pi$$
 (32)

If we combine (23) with the semiclassical approximation for the sums over eigenvalues

$$\sum_{n=-\infty}^{\infty} e^{iuE_n} \approx \sqrt{\frac{\pi}{u}} \int_{-\infty}^{\infty} dx e^{iux + i\pi/4} \frac{dV^{-1}(x)}{dx} = -i\sqrt{\pi u} \int_{-\infty}^{\infty} dx e^{iux + i\pi/4} V^{-1}(x)$$
 (33)

In order to obtain  $V^{-1}(x)$  from (24) we take the inverse Fourier transform, this involves the sum over Rieman Zeros  $\sum_{x} H(x-\gamma)(x-\gamma)^{-1/2}$ , if we put inside formula (32)

$$\frac{d^{1/2}H(x\pm u)}{dx^{1/2}} \approx H(x\pm u)(x\pm u)^{-1/2} \quad \text{with} \quad H(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases} \text{ and use the integral}$$

$$\int_{0}^{\infty} \frac{dx}{\sqrt{x}} e^{iux} = \sqrt{\frac{\pi}{u}} e^{i\pi/4}$$
 we find the desired result given in (29), so our inverse potential

 $V^{-1}(x)$  is in perfect agreement with the one given by Wu and Sprung, and also is compatible with the Riemann-Weyl expression (at least in distributional sense) relating Riemann Zeros and prime numbers. This inverse potential according to Riemann-Weyl formula plus the Zeta-regularized series (ignoring the divergent terms proportional to  $\varepsilon^{-k}$  as  $\varepsilon \to 0$ ) has an oscillating and an smooth part

$$\sum_{n=1}^{\infty} \frac{\Lambda(n)\cos(s\log n + \pi/4)}{\sqrt{n\log n}} \qquad \int_{-\infty}^{x} \frac{dt}{\sqrt{x-t}} \Re e^{\frac{\Gamma'}{L}} \left(\frac{1}{4} + \frac{it}{2}\right)$$
(34)

The first term can be regularized to give the Real part of  $\frac{d^{-1/2}}{ds^{-1/2}} \frac{\zeta'}{\zeta} \left( \frac{1}{2} + is \right)$  for any 's'

the second one is just the real part of  $\frac{d^{-1/2}}{ds^{-1/2}}\frac{\Gamma'}{\Gamma}\left(\frac{1}{4}+\frac{is}{2}\right)$ , in general since we are

interested in the Riemann Zeros  $\gamma_n$  as  $n \to \infty$  the smooth part can be approximated (for

big 'x') very well by the term 
$$\frac{d^{1/2}}{dx^{1/2}} \left( \frac{x}{2\pi} \log \frac{x}{2\pi} - \frac{x}{2\pi} \right)$$
, but in order our Hamiltonian

fulfills Riemann Hypothesis, also the oscillating part must be included into the potential, this is a fact that is ignored by Wu and Sprung, the inverse of the potential  $V^{-1}(x)$  can be simply obtained by imposing the Riemann-Weyl formula plus using the semiclassical approximation to relate a quantum mechanical Quantities (Energies, density of energies) to a pure classical quantity like the potential V(x). Also the formula

for the Energies 
$$\sum_{n} H(x - E_n) = \frac{1}{\pi} \arg \xi \left( \frac{1}{2} + i\sqrt{x} \right)$$
,  $\xi(s) = \frac{s(s-1)}{2} \Gamma\left( \frac{s}{2} \right) \pi^{-s/2} \zeta(s)$  is

just a consequence of the Riemann-Weyl formula, that stablishes a relationship between Riemann Zeros and prime numbers and that we have considered to be valid even in the distributional sense.

If we plug the function  $\pi\delta(r^2-s)=h(r,s)$ , s>0,inside the Riemann-Weyl formula, and use the Zeta regularization algorithm for the divergent series  $\sum_{n=1}^{\infty}\frac{\Lambda(n)}{\sqrt{n}}e^{i\sqrt{s}\log n}=_{reg}-\frac{\zeta'}{\zeta}\left(\frac{1}{2}+i\sqrt{s}\right) \text{ then Riemann-Weyl explicit formula gives the density of the Energies for the Hamiltonian } E_n=\gamma_n^2 \text{ as}$ 

$$\sum_{\gamma} \pi \delta \left( \gamma^{2} - s \right) =_{reg} \frac{\zeta}{\zeta} \left( \frac{1}{2} + i\sqrt{s} \right) \frac{1}{2\sqrt{s}} + \frac{\zeta'}{\zeta} \left( \frac{1}{2} - i\sqrt{s} \right) \frac{1}{2\sqrt{s}} + \frac{\zeta'}{\zeta} \left( \frac{1}{2} + i\sqrt{s} \right) \frac{1}{2\sqrt{s}} + \frac{\Gamma'}{\zeta} \left( \frac{1}{4} + i\frac{\sqrt{s}}{2} \right) \frac{1}{4\sqrt{s}} + \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} - i\frac{\sqrt{s}}{2} \right) \frac{1}{4\sqrt{s}} - \frac{\log \pi}{4\sqrt{s}} = \rho(s)$$

$$(35)$$

Where we have used the property of the Dirac delta function  $\delta(f(x)) = \sum_{x_n} \frac{\delta(x-x_n)}{|f'(x_n)|}$  with  $f(x_n) = 0$  inside (35). Integration over 's' gives the zeros counting function  $n(E) = \frac{1}{\pi} Arg \xi \left(\frac{1}{2} + i \sqrt{E}\right)$ , also if we approximated the sum  $\sum_{\gamma} \pi \delta(\gamma^2 - s)$  by an integral over the phase space  $\int_{V} \delta(E - H_2) dp dq$  in 1-D we find the Abel integral equation for the inverse of the potential  $\rho(E) = C \int_{0}^{E} \frac{du}{\sqrt{E-u}} \frac{dV_2^{-1}}{du}$ ,  $C \in R$ , a similar equation can be obtained using differentiation with respect to 'E' inside the Bohr-Sommerfeld quantization conditions.

Although we have considerEd an operator in the form  $-\partial_x^2 + V(x)$ , there exists a Liouville transform of variables that converts any second order Self-adjoint operator  $-\frac{d}{du}\left(p(u)\frac{dF}{du}\right) + q(u)F(u) - \lambda w(u)F(u)$  into an operator of the form  $-\partial_x^2 + V(x)$  by using a new redefinition of the dependent and independent variables by usign the Liouville transform:

$$x = \int_{u_0}^{u} dt \sqrt{\frac{w(t)}{p(t)}} \qquad V(x) = \left(w(x)p(x)\right)^{-1/4} \frac{d^2}{dx^2} \left(w(x)p(x)\right)^{1/4} - \frac{q(x)}{w(x)} \quad (36)$$

And  $\Psi(x) = (w(x)p(x))^{1/4} F(x)$ , also the operator in the form  $-\partial_x^2 + V(x)$  plus boundary condition is the easiest to work with, so we can apply the foundations of the Quantum mechanics to the case of the Riemann Hypothesis.

### APPENDIX A: FACTORIZATION OF A SECOND ORDER LINEAR DIFFERENTIAL OPERATOR INTO A PRODUCT OF TWO DIFFERENTIAL LINEAR OPERATORS.

From the theory of the Ajoint linear operators, is easy to prove that any second order differential linear operator  $-\partial_x^2 + V(x)$  can be expressed as the product

$$L_{+} = \frac{d}{dx} + A(x)$$
  $L_{-} = -\frac{d}{dx} + A(x)$  so  $-\partial_{x}^{2} + V(x) = L_{+}L_{-}$  and  $L_{+} = (L_{-})^{\dagger}$  (A.1)

Where the potential V(x) is related to the function 'A' by the Ricatti equation  $V(x) = \frac{dA}{dx} + A^2(x)$ , also the energies of  $-\partial_x^2 + V(x)$  will be Real (since the operator is Hermitian) and positive since

$$\langle \phi \mid -\partial_x^2 + V \mid \phi \rangle = \langle \phi \mid L_+ L_- \mid \phi \rangle = \langle \phi L_- \mid L_- \phi \rangle = || -\partial_x^2 + V \mid|_{\phi}^2 \ge 0 \tag{A.2}$$

Formula (A.2) tells us that for 1-D systems ALL the energies of the Hamiltonian will be Real (since it is a Hermitian operator) and positive, then it can not exist an Unbounded Hamiltonian operator in one dimension , for the case of our Hamiltonian whose Energies are the square of the imaginary part for the non-trivial zeros of the Riemann Zeta function  $-\partial_x^2 + V_2(x) = H_2$ ,  $E_n = \gamma_n^2$  then we have the auxiliar Eigenvalue equation  $(L\pm)f = \pm \frac{df}{dx} + A(x)f(x) = \pm i\gamma f(x)$ . If we introduce the cahnge of variable inside (A.1)  $x = \log u$  and put  $A = \frac{1}{2}$  the first term becomes the Theta operator  $\Theta_u = u \frac{d}{du}$ , if we also multiply all by  $-i\hbar$ , we find that  $-i\hbar L_+$  is just the Berry-Keating Hamiltonian  $-i\hbar L_+ = H_{BK} = -i\hbar \left(\frac{1}{2} + u \frac{d}{du}\right)$  whose Eigenvalues are the

imaginary parts of the Riemann Zeta zeros. The Theta operator appear inside the Berry-Keating Hamiltonian because it is conjectured that the imaginary part of the zeros can be obtained by the quantization of a dynamical system that violates time-reversal symmetry so  $\Theta_u(t,u(t)) \neq \Theta_u(-t,u(-t))$ , however for the square of the Berry-Keating (classical) Hamiltonian  $H_{bk}^2 = x^2 p^2$  the time reversal symmetry is conserved under the change  $t \to -t$ 

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