

# 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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- **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  $\frac{\xi\left(\frac{1}{2} + iE\right)}{\xi(1/2)} = \det(E - H)$  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, in order to get the boundary condition for our Quantum system  $\Psi(0) = 0$ , we impose the extra condition that for negative values of ‘x’ the potential becomes infinite (the particle can not penetrate in the regions whenever  $x < 0$  due to an infinite potential wall)  $V(x) = \infty$  for  $x < 0$ , then in the WKB approximation we have the fractional-differential equation.

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

Here we have introduced the fractional integral of order  $3/2$ , for a review about fractional Calculus we recommend the text by Oldham [11] 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

$$V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2} n(x)}{dx^{1/2}} \quad V^{-1}(x) = 2\sqrt{\pi} \frac{d^{-1/2} g(x)}{dx^{-1/2}} \quad \frac{dn}{dx} = g(x) = \sum_{n=0}^{\infty} \delta(x - E_n) \quad (3)$$

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  $[0, \infty)$  to check that our formula (3) can give coherent

results. In many cases (Harmonic oscillator) the quantization condition  $N(E) + \frac{1}{2}$  gives

better results than simply setting  $N(E)$  so our relation between the inverse of the potential and the counting function for states (Energies) of the 1-D Hamiltonian with a

general mass of 'm' takes the form  $V^{-1}(x) = \sqrt{\frac{2\pi\hbar^2}{m}} \frac{d^{1/2}}{dx^{1/2}} \left( \frac{1}{2} + n(x) \right)$ . This is a

consequence of the WKB quantization formula  $\int_C pdq = \left( n + \frac{1}{2} \right) \pi 2\hbar$ .

- *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  $\int_V D[\phi] e^{-\langle \phi | H | \phi \rangle} = \frac{1}{\sqrt{\det H}}$  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 assume Dirichlet boundary conditions on the interval  $[0, \infty)$

$$\frac{\det(H + z^2)}{\det(H)} = \frac{\prod_{n=0}^{\infty} (\lambda_n + z^2)}{\prod_{n=0}^{\infty} \lambda_n} = \prod_{n=0}^{\infty} \left( 1 + \frac{z^2}{\lambda_n} \right) = \frac{\Psi^{(z)}(L)}{\Psi^{(0)}(L)} \quad L \rightarrow \infty \quad (4)$$

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

$$\left( -\frac{d^2}{dx^2} + V(x) + z^2 \right) \Psi^{(z)}(x) = 0 \quad \Psi^{(z)}(0) = 0 \quad \frac{d\Psi^{(z)}(0)}{dx} = 1 \quad (5)$$

In the following section, we will discuss how to apply this theorem to evaluate functional determinants in one dimension plus the quantization condition

$N(E) = n(E) + \frac{1}{2}$  to obtain a Hamiltonian whose Energies are precisely the square of

the imaginary part of the Riemann zeros  $E_n = \gamma_n^2$  and so the functional determinant of

the Hamiltonian is the Riemann Xi-function 
$$\frac{\xi\left(\frac{1}{2} + i\sqrt{z}\right)}{\xi\left(\frac{1}{2}\right)} = \frac{\det(E-H)}{\det(-H)}$$
.

○ *Toy models of Functional determinants:*

As a toy model of this method, let be the Sturm-Liouville problem  $-\frac{d^2 y(x)}{dx^2} = E_n y(x)$  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

$$E_n = n^2 \pi^2 \quad n = 1, 2, 3, \dots \quad \frac{\sin(\sqrt{x})}{\sqrt{x}} = \prod_{n=1}^{\infty} \left(1 - \frac{x}{n^2 \pi^2}\right) \quad (6)$$

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

$$\frac{1}{x+i\varepsilon} = -i\pi\delta(x) + P\left(\frac{1}{x}\right) \quad \frac{\cot(x)}{2x} - \frac{1}{2x^2} =_{reg} \sum_{n=1}^{\infty} \frac{1}{x^2 - n^2 \pi^2 + i\varepsilon} \quad (7)$$

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

$$\frac{1}{\pi} \Im mg \left( \frac{\cot(x)}{2x} - \frac{1}{2x^2} \right) = - \sum_{n=1}^{\infty} \delta(x^2 - n^2 \pi^2)$$

making the substitution  $x \rightarrow \sqrt{E}$  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  $-\frac{d^2 y(x)}{dx^2} = E_n y(x)$  is given by the following formal formula

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

$(x-a)^{-1}$  (singular at the point a) by the distribution  $(x+i\varepsilon-a)^{-1}$  with  $\varepsilon \rightarrow 0$ , 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

$$N(E) = \frac{1}{\pi} Arg \xi \left( \frac{1}{2} + i\sqrt{E} \right)_{reg} = \frac{\xi'}{\xi} \left( \frac{1}{2} + \varepsilon + i\sqrt{x} \right) \frac{1}{2\sqrt{x}} = \sum_{n=0}^{\infty} \frac{a_n}{x+i\varepsilon-\gamma_n^2} \quad \{a_n\} \in R \quad (8)$$

Another more complicate example is the differential equation  $x \frac{d^2 y}{dx^2} + \frac{dy}{dx} + \lambda_n y = 0$

with the boundary conditions  $y(1) = 0$  and with a solution bounded as  $x \rightarrow 0$ , 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

$$J_0(\sqrt{x}) = J_0(0) \prod_{n=0}^{\infty} \left( 1 - \frac{x}{\alpha_n^2} \right), \text{ in case Riemann Hypothesis is true (and the self-adjoint}$$

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

## 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  $N(E) = \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{E} \right)$  (since now we are counting squares of the Riemann zeros), using the same reasoning we did in (3) 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 as the following expression.

$$V_2^{-1}(x) \approx 2\sqrt{\pi} \frac{d^{1/2}}{dx^{1/2}} \left( \frac{1}{2} + \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + \varepsilon + i\sqrt{x} \right) \right) \quad \varepsilon \rightarrow 0 \quad x > 0 \quad (9)$$

In this case the functional determinant of this Hamiltonian should be

$$\frac{\det(H_2 - z)}{\det(H_2)} = \frac{\prod_{n=0}^{\infty} (E_n - z)}{\prod_{n=0}^{\infty} E_n} = \prod_{n=0}^{\infty} \left( 1 - \frac{z}{\gamma_n^2} \right) = \frac{\xi(1/2 + i\sqrt{z})}{\xi(1/2)} \quad z > 0 \quad (10)$$

In this case the Hamiltonian would be bounded so  $\langle H_2 \rangle \geq \gamma_0^2 = 199.750490..$  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

$$\frac{\det(H_2 - z)}{\det(H_2)} = \frac{\Psi^{(z)}(L)}{\Psi^{(0)}(L)} \text{ with } \quad \left( -\partial_x^2 + V_2(x) - z \right) \Psi^{(z)}(x) = 0 \quad (11)$$

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

Unfortunately , equation (8) can not be solved exactly , and we will have to use the WKB approximation in order to obtain the function  $\Psi^{(z)}(x)$

$$\Psi^{(z)}(x) \approx (z - V_2(x))^{-1/4} \left\{ C_+ \exp\left(i \int_0^x \sqrt{z - V_2(t)} dt\right) + C_- \exp\left(-i \int_0^x \sqrt{z - V_2(t)} dt\right) \right\} \quad (12)$$

$C_+ + C_- = 0$  since  $\Psi^{(z)}(0) = 0$ . Another equivalent formulation of Gelfand-Yaglom theorem applied to Riemann Hypothesis would include the quotient of 2 functional determinants

$$\frac{\det(-\partial_x^2 + V_2 - z)}{\det(-\partial_x^2 + V_0 - z)} = \frac{\Psi^{(z)}(L)}{\Psi_{free}^{(z)}(L)} = \frac{\xi\left(\frac{1}{2} + i\sqrt{z}\right)}{\xi(1/2)} \quad L \rightarrow \infty, V_0 = 0 \quad (13)$$

With the initial conditions,  $\Psi^{(z)}(0) = 0 = \Psi_{free}^{(z)}(0)$  and  $\frac{d\Psi^{(z)}(0)}{dx} = 1 = \frac{d\Psi_{free}^{(z)}(0)}{dx}$

(Also if we add a term  $\frac{1}{4}$  to the potential  $V_2(x)$  inside (14) then the eigenvalues would 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  $\varepsilon \rightarrow 0$  (given in (14) in an equivalent form) 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  $\sin(\sqrt{x})$ ,  $J_0(\sqrt{x})$ . 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  $f(x)$ .

○ *Inverse of the Potential for  $x > 0$ ,  $x = 0$  and  $x < 0$ :*

Since (9) is only valid for positive 's' what happens for  $s \leq 0$ ?, the idea is that for negative E (or s) the Eigenvalue counting function  $N(E) = \sum_{\gamma^2 \leq E} 1$  is equal to 0 (there are no negative eigenvalues) in this case the equation for the inverse potential and the potential turn out to be of the following form

$$V^{-1}(x) = \begin{cases} \frac{2}{\sqrt{\pi}} \frac{d^{1/2}}{dx^{1/2}} \left( Arg \xi\left(\frac{1}{2} + i\sqrt{x}\right) + \frac{1}{2} \right) & x > 0 \\ 0 & x \leq 0 \end{cases} \quad \text{so } V(x) = 0 \text{ for } x \leq 0 \quad (14)$$

And for positive 'x' we have to invert the function  $2\sqrt{\pi} \frac{d^{1/2}}{dx^{1/2}} \left( \frac{1}{2} + \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{x} \right) \right)$ , from (36) we get that there is a potential barrier at  $x=0$  so we must impose the eigenvalue conditions for our Schrödinger equation as  $y(0) = 0 = y(\infty)$ .

From equation (14) and after inversion, we will get that for negative 'x' there is an infinite potential barrier so  $V(x) = \infty$  for  $x < 0$ , so the wave function of the system is 0 at  $x=0$ , this is not the unique possibility another alternative is to consider that the potential is EVEN  $V(x) = V(-x)$  in this case the density of states will be a slightly different and the inverse of the potential will be defined for every 'x' in the form

$$V^{-1}(x) \approx \sqrt{\pi} \frac{d^{1/2}}{dx^{1/2}} \left( \frac{1}{2} + \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{x} \right) \right),$$

in this case there are 2 inverses, we must take the one with  $V(x) \geq 0$   $x \in R$ , so all the energies are positive

$\langle H \rangle_\phi = E_n > 0$ . However if we make the potential 'even'  $V(x) = V(-x)$  the eigenfunctions will be odd or even  $\Psi_n(x) = \Psi_n(-x)(-1)^n$  and for even Eigenfunctions we can not warrant that  $\Psi(0) = 0$  so we are losing a boundary condition.

o *Riemann Weyl formula, Primes Riemann zeros and the inverse of  $V_2^{-1}(x)$ :*

In Analytic Number Theory there is a formula now named the Riemann-Weyl formula, relating a sum over primes and prime powers to a sum involving the imaginary part of the Riemann zeros

$$\sum_{\gamma} h(\gamma) = 2h\left(\frac{i}{2}\right) - 2 \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} g(\log n) + \frac{1}{2\pi} \int_{-\infty}^{\infty} dr h(r) \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} + \frac{ir}{2} \right) - g(0) \log \pi \quad (15)$$

If we insert inside ( ) the function  $h(r, s) = \delta(s - r^2)$  and use the Zeta regularization algorithm to avoid the problem that the first sum on the right of ( ) is divergent

$$\sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} e^{i\sqrt{s} \log n} =_{reg} - \frac{\zeta'}{\zeta} \left( \frac{1}{2} + i\sqrt{s} \right)$$

$$\begin{aligned} \sum_{\gamma} \pi \delta(\gamma^2 - s) &=_{reg} \frac{\zeta'}{\zeta} \left( \frac{1}{2} + i\sqrt{s} \right) \frac{1}{2\sqrt{s}} + \frac{\zeta'}{\zeta} \left( \frac{1}{2} - i\sqrt{s} \right) \frac{1}{2\sqrt{s}} - \frac{\log \pi}{2\sqrt{s}} \\ &+ \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} + i\frac{\sqrt{s}}{2} \right) \frac{1}{4\sqrt{s}} + \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} - i\frac{\sqrt{s}}{2} \right) \frac{1}{4\sqrt{s}} = \rho(s) \end{aligned} \quad (16)$$

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

$$n(E) = \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{E} \right),$$

also if we approximated the sum  $\sum_{\gamma} \pi \delta(\gamma^2 - s)$  by an

integral over the phase space  $\int_V \delta(E - H_2) dpdq$  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.

o *Smooth and oscillating part of the inverse  $V_2^{-1}(x)$  :*

Also if we make use of the Zeta regularization technique and the Riemann-Von Mangoldt formulae [ ], for big positive  $-x$  the inverse of the potential can be written as

$$V_2^{-1} \approx 2\sqrt{\pi} \frac{d^{1/2}}{dx^{1/2}} \left( \frac{1}{2} + N_{smooth}(x) + N_{oscillating} \right), \text{ with}$$

$$N_{smooth}(x) = \frac{1}{\pi} \text{Arg} \frac{\Gamma'}{\Gamma} \left( \frac{1}{4} + i\sqrt{x} \right) - \frac{\sqrt{x}}{2\pi} \approx \frac{\sqrt{x}}{2\pi} \log \left( \sqrt{\frac{x}{4\pi^2}} \right) - \frac{\sqrt{x}}{2\pi} + \frac{7}{8} + O\left(\frac{1}{\sqrt{x}}\right) \quad (17)$$

(This smooth density of states fullfills Weyl's law with dimension  $d = 1 + \varepsilon$  (due to the logarithmic term inside the asymptotics) namely  $N_{smooth}(E) \approx O(E^{d/2})$  )

$$N_{oscillating}(x) = \frac{1}{\pi} \text{Arg} \zeta \left( \frac{1}{2} + i\sqrt{x} \right) \approx \sum_{n=2}^{\infty} \frac{\Lambda(n)}{\log n} \frac{1}{\pi} \frac{\sin(\sqrt{x} \log n + \pi)}{\sqrt{n}} \quad x > 0 \quad (18)$$

The last Fourier series is DIVERGENT, in order to obtain a correction to the smooth part of the inverse of the potential, we could approximate this sum by using only the first 10 20 or 100 primes in order to obtain a finite correction to the smooth part, the idea is that for big 'x' and in the sense of distribution theory the inverse of the potential

should be almost equal to  $V_2^{-1} \approx A \sum_{n=0}^{\infty} H(x - E_n) (x - E_n)^{-1/2}$  for some real A. The

Fourier series inside (18) is divergent, so perhaps we can take only the first 10 20 or 100 first primes in order to obtain a finite result for (18).

Then by the Gelfand-Yaglom theorem the functional determinant of  $Det(E - H_2)$  with energies  $E - \gamma_n^2$  will be proportional to the Riemann Xi-function on the critical line

$$\prod_{i=0}^{\infty} (E - \gamma_i^2) \approx \xi \left( \frac{1}{2} + i\sqrt{E} \right), \text{ this determinant can be obtained by solving the initial}$$

value problem  $(-\partial_x^2 + V_2(x) - z)\phi(z, x) = 0$  with  $\partial_x \phi(z, 0) = 1$ ,  $\phi(z, 0) = 0$

So, from our method we can deduce that

a) The Eigenvalue counting function  $N(E) = \sum_{E_n \leq E} 1 = \sum_{n=0}^{\infty} H(E - E_n)$  with  $E_n = \gamma_n^2$ ,

is proportional to  $\frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{x} \right)$  by using Riemann-Weyl formula



b) The inverse of the potential inside  $-\partial_x^2 + V_2(x) = H_2$  is proportional to the half-derivative of  $N(E) = \sum_{n=0}^{\infty} H(E - E_n)$ , this is obtained by WKB analysis.

c) The factor  $N(E) = \sum_{n=0}^{\infty} H(E - E_n)$  can be approximated by the sum  $N(E) = N_{smooth}(E) + N_{oscillating}(E)$ , the smooth part obeys an asymptotic law called Weyl's law, namely  $N_{smooth}(E) = O(E^{1/2+\epsilon})$  for any real and positive epsilon, the oscillating part can be approximated by truncation of the divergent

$$\text{Fourier series } \sum_{n=2}^{\infty} \frac{\Lambda(n)}{\log n} \frac{1}{\pi} \frac{\sin(\sqrt{x} \log n + \pi)}{\sqrt{n}}$$

d) The quotient of the two functional determinants  $Det(E - H_2)$  and  $Det(-H_2)$  will be proportional (for  $E > 0$ ) to the function  $\xi\left(\frac{1}{2} + i\sqrt{E}\right)$ , with

$$-\partial_x^2 + V_2(x) = H_2 \quad \text{and} \quad V_2^{-1} \approx 2\sqrt{\pi} \frac{d^{1/2}}{dx^{1/2}} \left( \frac{1}{2} + N(x) \right)$$

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

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 should work ?:*

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

$$\text{(Half)- Harmonic oscillator } V = \frac{(\omega x)^2}{4} \quad N(E) = \frac{E}{2\omega} \quad V^{-1}(x) = \frac{2\sqrt{E}}{\omega} \quad (19)$$

$$\text{Linear potential } V = kx \quad N(E) = \frac{2E^{3/2}}{3\pi k} \quad V^{-1}(x) = \frac{x}{k} \quad (20)$$

$$\text{Infinite potential well } V = 0 \quad N(E) = \frac{\sqrt{E}}{\pi} \quad V^{-1}(x) = 1 \quad (21)$$

(We assume that in (19) (20) and (21) the potential  $V(x) = \infty$   $x < 0$  )

In all cases and for simplicity we have used the notation  $\hbar = 2m = 1 = L$  , here ‘L’ is the length of the well inside (21) , (19) and (20) are correct results that one can obtain using the exact Quantum theory , (21) 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

$$\frac{d^{1/2} E^k}{dE^{1/2}} = \frac{\Gamma(k+1)}{\Gamma(k+1/2)} E^{k-1/2} \quad [11] ,$$

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  $V(x) = \begin{cases} Cx^m & x \geq 0 \\ \infty & x < 0 \end{cases}$  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)

$$N(E) = \frac{C^{-\frac{1}{m}}}{\sqrt{4\pi}} \cdot \frac{\Gamma\left(\frac{1}{m}+1\right)}{\Gamma\left(\frac{1}{m}+\frac{3}{2}\right)} E^{\frac{1}{m}+\frac{1}{2}} ,$$

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 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  $V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2} \pi(x)}{dx^{1/2}}$  , 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

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

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

$$\frac{\xi'}{\xi}\left(\frac{1}{2}+i\sqrt{z}\right) \frac{1}{2\sqrt{z}} = \sum_{n=0}^{\infty} \frac{a_n}{z+i\varepsilon-\gamma_n^2} \quad a_n = \operatorname{Re} s \left( z = \gamma_n, \frac{\xi'}{\xi} \right) \quad (22)$$

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

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

$$g(E) = \frac{1}{\pi} \Im m \partial_E \log \xi \left( \frac{1}{2} + iE \right) = - \sum_{n=-\infty}^{\infty} \delta(E - \gamma_n) \quad (23)$$

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

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

$$\sum_{\gamma} f(\gamma) = -\frac{1}{\pi} \int_0^{\infty} ds f'(s) \text{Arg} \xi \left( \frac{1}{2} + is \right) \quad -\frac{\zeta'}{\zeta} \left( \frac{1}{2} + iz \right) = \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} e^{is \log n} \quad (24)$$

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

$$\sum_{\gamma} f(\gamma) = 2f\left(\frac{i}{2}\right) - g(0) \log \pi - 2 \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} g(\log n) + \frac{1}{2\pi} \int_{-\infty}^{\infty} ds f(s) \frac{\Gamma'(s)}{\Gamma\left(\frac{1}{4} + \frac{is}{2}\right)} \quad (25)$$

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

$$2p = \dot{x} \quad \dot{p} = -\frac{\partial V}{\partial x} \quad n(E) = \frac{1}{\pi} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{E} \right) \quad V^{-1}(x) = 2\sqrt{\pi} \frac{d^{1/2} n(x)}{dx^{1/2}} \quad (26)$$

Then the Gutzwiller trace for this dynamical one dimensional system (x,t) is

$g(E) = g_{smooth}(E) + \sum_{n=1}^{\infty} \frac{\Lambda(n)}{\sqrt{n}} \cos(E \log n)$ , for big E the smooth part can be

approximated by  $g_{smooth}(E) \approx \frac{\log E}{2\pi}$ . 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 Schrödinger 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

$V_2^{-1}(x) \approx \frac{2}{\sqrt{\pi}} \frac{d^{1/2}}{dx^{1/2}} \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{x} \right)$  we may use the Grunwald-Letnikov definition of the half-derivative to write the inverse of the potential in the form

$$V_2^{-1}(x) \approx \frac{2}{\sqrt{\pi\varepsilon}} \sum_{m=0}^{\infty} \binom{1/2}{m} (-1)^m \text{Arg} \xi \left( \frac{1}{2} + i\sqrt{x + \left(\frac{1}{2} - m\right)\varepsilon} \right) \quad (27)$$

Here ‘ $\varepsilon$ ’ is a 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

(27) 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 (27) across the line  $y = x$  to get the numerical values for the potential  $V_2(x_j)$ , we have solved numerically the Schrödinger 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  $(-\partial_x^2 + f(x) - z)y_z(x) = 0$  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  $\xi \left( \frac{1}{2} + i\sqrt{z} \right) = \xi \left( \frac{1}{2} \right) \prod_{n=0}^{\infty} \left( 1 - \frac{z}{\gamma_n^2} \right) = \frac{y_{(z)}(L)}{y_{(z)free}(L)} \quad L \rightarrow \infty$

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 using the Liouville transform:

$$x = \int_{u_0}^u dt \sqrt{\frac{w(t)}{p(t)}} \quad V(x) = (w(x)p(x))^{-1/4} \frac{d^2}{dx^2} (w(x)p(x))^{1/4} - \frac{q(x)}{w(x)} \quad (28)$$

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

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

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

$$\langle \phi | -\partial_x^2 + V | \phi \rangle = \langle \phi | L_+L_- | \phi \rangle = \langle \phi L_- | L_- \phi \rangle = \| -\partial_x^2 + V \|^2_\phi \geq 0 \quad (\text{A.2})$$

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  $t \rightarrow -t$ , the commutator of the 2 ladder operators involved in our definition of

the Hamiltonian is  $[L_+, L_-] = 2 \frac{dA}{dx}$  it only vanishes for the case of the A being a

constant function of 'x', for example in a Berry-Keating model.

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