# Out-of-Time-Order Correlator of Berry-Keating model

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*by*

**Roll: 106712**

**Registration: 2016-514-722**


**University of Dhaka**

**Dhaka - 1000**

**Abstract**

Berry-Keating Hamiltonian $H_0 = \frac{1}{2}(xp + px)$ resembles the Hilbert-Pólya conjecture of Riemann Hypothesis shows quantum chaotic behavior. In this paper we first quantize $xp$ and $1/xp$ and achieve the same spectrum with minor phase addition. We observe quantize $xp$ and add boundary conditions to evaluate the spectrum with proper eigenfunction. Then we measured the Out-of-Time-Order Correlator (OTOC) of the Hamiltonian,to measure the quantum chaos of the Hamiltonian.

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# Chapter 1

# Introduction

The classical zeta/ Riemann zeta function defined as $\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$[1], where s is $s = \sigma + it$ and n is the integers. If the real part of s is greater than 1 (Re $s > 1$), the zeta function converges. But at real part equal to 1 (Re $s = 1$) it becomes the harmonic series $\zeta(1) = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + ....$ and diverges. So there begs the question where does the zeta fucntion goes to zero. It was found that there are two types of condition that make the Riemann zeta function which is called Riemann zero or Zeta zero. For negetive integers($n = -2, -4, -6, .....$) in the Riemann zeta function becomes zero. These types of zeros are called Trivial zeros. And the other kind of zeros, which are called Non-Trivial zeros, lie between real part of s in Re $0 < s < 1$. Riemann hypothesize that all the non-trivial zeros lie at $s = \frac{1}{2}$. This is the famous Riemann hypothesis. Euler showed that the existing classical zeta function has a connection to the product of all prime numbers.

He proved that $\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \frac{1}{1-p^{-s}}$ where p is the primes. So if anyone can prove the Riemann hypothesis, they can also prove that all the prime numbers must be lies the line of Re $s = \frac{1}{2}$.It is generally agreed upon that the Riemann Hypothesis is the single most important topic in Analytic Number Theory[2, 3, 4, 5].Hilbert-P*ó*lya sugested that the imaginary part of the s in the Non-Trivial zeros will be a self-adjoint oprator[6, 7, 8]. So the s will more look like as $s = \sigma - iE_n$.The work done by Selberg in the 1950s, in which he discovered a surprising duality between the eigenvalues of the Laplacian acting on Riemann surfaces with constant negative curvature and the length spectrum of their geodesics [9], is likely what provided the first clue of the sufficiency of this conjecture. In this work, Selberg observed that there was a relationship between the two. This link is made possible by the Selberg trace formula, which has a striking resemblance to the Riemann explicit formula. Another significant clue was provided in 1973 by the work of Montgomery, who, on the assumption that the RH was true, demonstrated that the Riemann zeros are distributed in accordance with the Gaussian Unitary Ensemble statistics of random matrix models [10]. This was a very helpful piece of information. In the 1980s, Odlyzko obtained some very spectacular numerical discoveries, which supported the conclusions that Montgomery had drawn [11]. Berry-Keating took this suggestion and proposed that the self-adjoint operator, which is $E_n$, will be a Hamiltonian which is $\hat{H} = \frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})$. Berry-Keating also proposed that this Hamiltonian shows quantum chaotic behaviour. One can tell if any object is in chaos or chaotic

behavoiur is sensitive dependece of initial condition, or we can say that a particle forget its memory about its initial condition. If a equation of a system is non-linear ODE, the system is chaotic or in chaos. Which can be describe in the following statement. Let there are two partiticle at a distance seperated by $\delta x$ at time $t = 0$ or $\delta x(0)$ and after some time $t$ the distance between the particle $\delta x(t)$, the relation of the initial and the final posotion of a chaotic system is $|\delta x(t)| \approx e^{t\lambda}|\delta x(0)|$, where t is time and $\lambda$ is the Lyapunov exponent. Lyapunov exponent measures the sensitivity of initial condition.

In this paper we took the Berry-Keating Hamiltonian and also look at the Connes approach to the same Hamiltonian for evaluation of semiclassical states.[12, 13, 1] And also we look at German Sierra approach.[14]Berry and Keating used a Planck cell regularization, in which the smooth component of the Riemann zeros is represented semiclassically as discrete energy levels. Connes, on the other hand, chose an upper cutoff for the position and momenta, resulting in a semiclassical continuous spectrum devoid of smooth zeros, which all include in the paper. They both consider x and p are the 1D location and momentum of the particle. German Sierra took both of the regularization, Berry-Keating and Connes regularization and took assumption only on x or bounds x and excludes p.

Out-of-Time-Order Correlator is the mesurement of chaos of quantum system. It was first introduced in a calculation of a vertex correction of a current for a superconductor[15]. The out-of-time-order correlator (OTOC) is typically defined by [16]

$$C_T \equiv -\left\langle [W(t), V(0)]^2 \right\rangle \tag{1.1}$$

where $< \cdots >$ represents the thermal average. W(t) and V(t) are operators as time in t in the Heisenberg representation. The OTOC, first introduced in a calculation of a vertex correction of a current for a superconductor[15], was recently turned out to be considered as a measure of the magnitude of quantum chaos. A naive argument for the relation between the OTOC and chaos is as follows[14]. Consider position and momentum operators, x(t) and p(t), in a quantum system. We can define an OTOC as $C_T = -\left\langle [x(t), p(0)]^2 \right\rangle$. Taking a naive semiclassical limit, we would be able to replace the commutator $[x(t), p(0)]$ by the Poissoin bracket $i\hbar\{x(t), p(0)\}_{PB} = i\hbar\frac{\delta x(t)}{\delta x(0)}$. For a classically chaotic system with a Lyapunov exponent $\lambda$, we have $\frac{\delta x(t)}{\delta x(0)} \sim e^{\lambda t}$ because of sensitivity to initial condition. Thus, the OTOC should grow as $\sim \hbar^2 e^{2\lambda t}$ and we can read off the quatnum Lyapunov exponent $\lambda$ form it. The quantization of a classically chaotic system may provide a positive quanutm Lyapunov exponent of the OTOC. Historically, the nearest neighbour distribution (NND) for the energy level spectrum has been used to quantify quantum chaos [17]. For integrable and non-integrable systems, it is considered that NNDs are given by Poission and Wigner distributions. The OTOC is expected to be another measure of quantum chaos. A possible distinction from the classical chaotic system is that the OTOC does not grow eternally but saturates at the Ehrenfest time $t_E$. The Ehrenfest

time is defined by the time scale beyond which the wave function spreads over the whole system. It is roughly characterized as a boundary between a particle-like behavior and a wave-like behavior of the wave function.

In the context of AdS/CFT correspondence [18] or quantum gravity, the OTOC has gained prominence in recent years as a crucial observable. In [19], an upper bound of 2kB T / was proposed for the qua- ntum Lyapunov exponent. Black hole horizon quantum information is where the bound was first proposed [20, 21] (see also references [22, 23, 24, 25, 26]). Infinitely long range dis-order interactions between Majorana fermions in the quantum mechanics of the Sachdev-Ye-Kitaev (SYK) model [27, 28] saturate the Lyapunov bound. The SYK model depicts a quantum black hole through the AdS/CFT correspondence after the quantum Lyapunov constraint is saturated.

In the definition of OTOC, we consider the thermal average of $-\left\langle [W(t), V(0)]^2 \right\rangle$. When we take thermal average, we need to consider the four point operator $\left\langle [W(t), V(0)]^2 \right\rangle$ instead of two point operator $\langle [W(t), V(0)] \rangle$. The reason is as follows. Assuming that we can replace the commutator by Poission bracket by semiclassical limit, $\langle [W(t), V(0)] \rangle$ would also show the exponential growth $\sim e^{\lambda t}$. However, its coefficient can be both positive and negetive. By taking the thermal average, their contributions would be canceled. From the quantum theory point of view, $\langle [W(t), V(0)] \rangle$ measures the correlation between W(t) and V(0). Therefore, the two point function decays as $t \to \infty$ and cannot show the chaotic behavior.

Now we look into the Berry-Keating and Connes semiclassical approaches

to $H = xp$

# Chapter 2

# Semiclassical approach

The classical Berry-Keating-Connes (BKC) Hamiltonian is[12, 29]

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

which has hyperbolic trajectories

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

So the dynamics is unbounded. There is a continuous spectrum as the quantum level. Berry-Keating and Connes introduced two different types of reularizations and counted the semiclassical states. Berry-Keating introduced Plank cell in a phase space: $|x| > l_x$ and $|p| > l_p$, with $l_x l_p = 2\pi\hbar$. Connes choosed $|x| < \Lambda$ and $|p| < \Lambda$, where $\Lambda$ is a cutoff. German Sierra introduced us a third regularization, $l_x < x < \Lambda$ combines the Berry-Keating

and Connes regularization position, not taking assumptions for the momenta p.

Semiclassical states number $\mathcal{N}(E)$ with an enery between 0 to E is given by

$$\begin{aligned} \mathcal{N}(E) &= \frac{A}{2\pi\hbar} \\ &= \frac{A}{h} \end{aligned} \tag{2.3}$$

Where A is the area of the allowed phase space region below the curve $E = xp$.

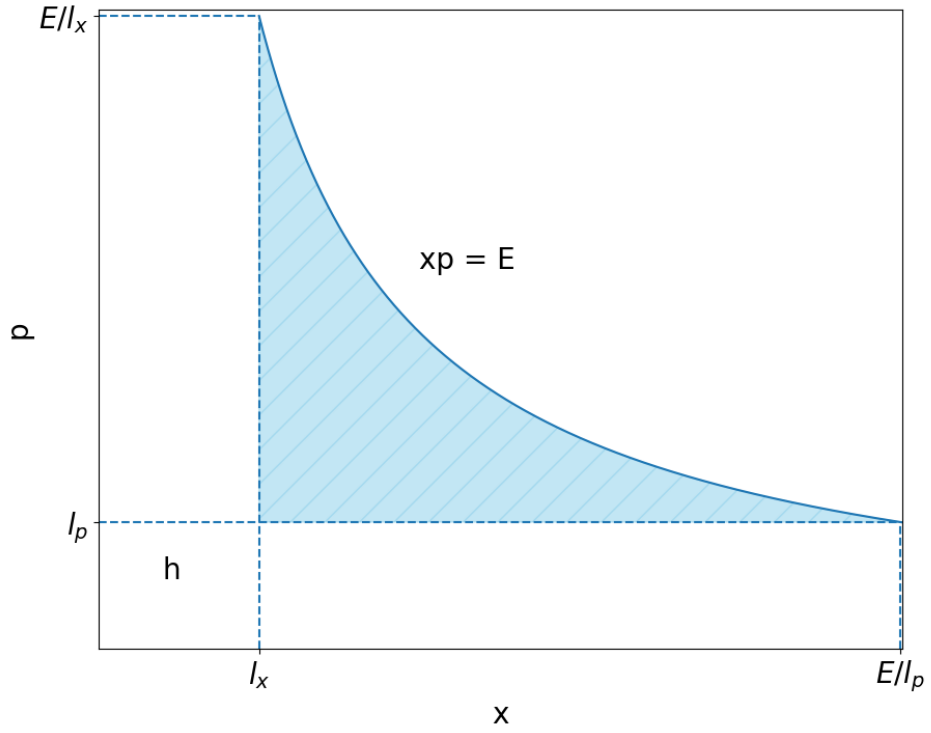


Figure 2.1: Berry-Keating Regularization

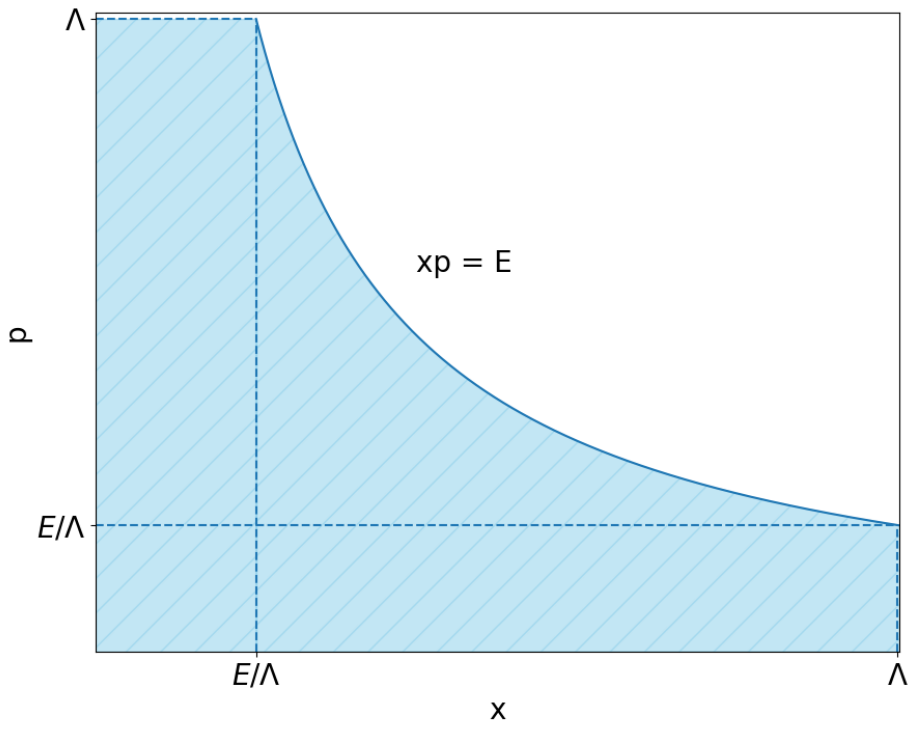


Figure 2.2: Connes Regularization

So the the number of semiclassical states will be for Berry-Keating regu-

larization

$$\begin{aligned}
\mathcal{N}_{BK}(E) &= \frac{1}{h}\int_{l_x}^{\frac{E}{l_p}} dx \int_{l_p}^{\frac{E}{x}} dp + ..... \\
&= \frac{1}{h}\left[\int_{l_x}^{\frac{E}{l_p}} dx \left[\frac{E}{x} - l_p\right]\right] \\
&= \frac{1}{h}\left[E\left[\ln x\right]_{l_x}^{\frac{E}{l_p}} - l_p\left[\frac{E}{l_p} - l_x\right]\right] \\
&= \frac{1}{h}\left[E\ln\frac{E}{l_x l_p} - E - l_x l_p\right] \\
&= \frac{1}{h}\left[E\ln\frac{E}{l_x l_p} - E - h\right] \\
&= \frac{E}{h}\left[\ln\frac{E}{l_x l_p} - 1\right] + 1 \\
&= \frac{E}{2\pi\hbar}\left[\ln\frac{E}{2\pi\hbar} - 1\right] + 1
\end{aligned} \tag{2.4}$$

adding Maslov phase $(-\frac{1}{8})$ and $\hbar = 1$, it becomes

$$\mathcal{N}_{BK}(E) = \frac{E}{2\pi}\left[\ln\frac{E}{2\pi} - 1\right] + \frac{7}{8} + ....., \qquad E >> 1 \tag{2.5}$$

The exact formula for the Riemann zeros, $\mathcal{N}_R(E)$ contains a fluctuation term which depends on the zeta funcion.[1]

$$\begin{aligned}
\mathcal{N}_R(E) &= \langle\mathcal{N}\rangle + \mathcal{N}_{fl}(E) \\
\langle\mathcal{N}(E)\rangle &= \frac{1}{\pi} Im\ ln\left[\Gamma\frac{1}{2}\left(\frac{1}{2} - iE\right)\right] - \frac{E}{2\pi} ln\pi + 1 \\
\mathcal{N}_{fl}(E) &= \frac{1}{\pi} Im\ ln\left[\zeta\left(\frac{1}{2} - iE\right)\right]
\end{aligned} \tag{2.6}$$

Bery-Keatin took this result and analogies between formulae in Nunber Theory and Quantum Chaos, they pointed the quantization of classical chaotic Hamiltonian give rise to the zeros as point like spectra.[12, 30] Whereas Connes found the number of semicassical states diverges in the limit where the cutoff $\Lambda$ goes to infinity, and that therre us a finite size correction given by mins the average position of the Riemann zeros.

$$\begin{aligned}
\mathcal{N}_c(E) &= \frac{1}{h}\left[2E - \left(\frac{E}{\Lambda}\right)^2 + \int_{\frac{E}{\Lambda}}^{\Lambda} dx \int_{\frac{E}{\Lambda}}^{\frac{E}{x}} dp\right] \\
&= \frac{1}{h}\left[2E - \left(\frac{E}{\Lambda}\right)^2 + \int_{\frac{E}{\Lambda}}^{\Lambda} dx \left[\frac{E}{x} - \frac{E}{\Lambda}\right]\right] \\
&= \frac{1}{h}\left[2E - \left(\frac{E}{\Lambda}\right)^2 + E\left[ln\ x\right]_{\frac{E}{\Lambda}}^{\Lambda} - \frac{E}{\Lambda}\left[\Lambda - \frac{E}{\Lambda}\right]\right] \\
&= \frac{1}{h}\left[2E - \left(\frac{E}{\Lambda}\right)^2 + E\left[ln\ \frac{\Lambda^2}{E}\right] - E + \left(\frac{E}{\Lambda}\right)^2\right] \\
&= \frac{1}{h}\left[E + E\left[ln\ \frac{\Lambda^2}{E}\right]\right] \\
&= \frac{1}{h}\left[E + E\left[ln\ \frac{\Lambda^2}{E}\frac{2\pi}{2\pi}\right]\right] \\
&= \frac{E}{h} ln\ \frac{\Lambda^2}{2\pi} - \frac{E}{h}\left[ln\ \frac{E}{2\pi} - 1\right] \\
&= \frac{E}{2\pi} ln\ \frac{\Lambda^2}{2\pi} - \frac{E}{2\pi}\left[ln\ \frac{E}{2\pi} - 1\right] \qquad [taking \quad \hbar = 1]
\end{aligned} \tag{2.7}$$

This result les to the missing spectral interpretation of the Riemann zeros, according to which there is a continuum of eginstates (represented by the term $\frac{E}{\pi} ln\ \Lambda$ in $\mathcal{N}(E)$) where states asscoiated with Riemann zeros are

missing.

Finally, in the S-regularization the number of semiclasical states diverges as $\frac{E}{2\pi}\ ln\ \frac{\Lambda}{l_x}$ suggesting a continuum spectrum, like in Connes's approach. But there is no finite size correction to that formula, and cosequently the possible connection to the Riemann zeros is lost.

Table 2.1:
Three different regularizations of $H = xp$ and the corresponding number of semiclassical states in units $\hbar = 1$[31]

| Type | Regularization | $\mathcal{N}(E)$ |
|---|---|---|
| BK | $\|x\| > l_x, \|p\| > l_p$ | $\frac{E}{2\pi}\left(ln\ \frac{E}{2\pi} - 1\right) + 1$ |
| C | $\|x\| < \Lambda, \|p\| < \Lambda$ | $\frac{E}{2\pi} ln\ \frac{\Lambda^2}{2\pi} - \frac{E}{2\pi}\left(\ln\ \frac{E}{2\pi} - 1\right)$ |
| S | $l_x < x < \Lambda$ | $\frac{E}{2\pi} ln\ \frac{\Lambda}{l_x}$ |

# Chapter 3

# Quantization of xp and $\frac{1}{xp}$

## 3.1 The Hamitoninan $H_0 = xp$

Here we construst a self adjoint operator $H_0$ which acts on a Hilbert space $L^2(a,b)$ of square integrable function in the interval $(a,b)$. Taking $x \geqslant 0$ , there are four possible intervals: $a = 0, l_x$ and $b = \Lambda, \infty$ where $l_x$ and $\Lambda$ were introduced (we shall take $l_x$ and $\Lambda = N > 1$). Berry-Keating defined the quantum Hamiltonian $H_0$ as the normal ordered expresion

$$H_0 = \frac{1}{2}(xp + px) \tag{3.1}$$

where $p = -i\hbar\frac{d}{dx}$. If $x \geqslant 0$, Eq. (3.1) is equivalent to

$$\begin{aligned} H_0 &= \sqrt{x}p\sqrt{x} = -i\hbar\sqrt{x}\frac{d}{dx}\sqrt{x} \\ &= -i\hbar\left(x\frac{d}{dx} + \frac{d}{dx}x\right) \end{aligned} \tag{3.2}$$

We know that the canonical commutation relation is

$$[\hat{x}, \hat{p}] = i\hbar \tag{3.3}$$

or, (dropping hat cause we're dealing with quantum system and operators)

$$\begin{aligned} [x, p] &= i\hbar \\ \implies \left[x, -i\hbar\frac{d}{dx}\right] &= i\hbar \\ \implies -i\hbar\left[x, \frac{d}{dx}\right] &= i\hbar \\ \implies \left[x, \frac{d}{dx}\right] &= -1 \\ \implies x\frac{d}{dx} - \frac{d}{dx}x &= -1 \\ \implies \frac{d}{dx}x &= x\frac{d}{dx} + 1 \end{aligned} \tag{3.4}$$

Taking this value to R.H.S of Eq(3.2)

$$\begin{aligned} -i\hbar\left(x\frac{d}{dx}+\frac{d}{dx}\right)f &= -i\hbar\left[2x\frac{d}{dx}+1\right] \\ &= -i\hbar 2x\left[\frac{d}{dx}+\frac{1}{x}\frac{1}{2}\right]f \\ &= -i\hbar\frac{1}{\sqrt{x}}\frac{d}{dx}\left(\sqrt{x}f\right) \\ &= -i\hbar\frac{1}{\sqrt{x}}\frac{d}{dx}\left(\sqrt{x}f\right) \\ &= \frac{1}{\sqrt{x}}\left(-i\hbar\frac{d}{dx}\right)\sqrt{x}f \end{aligned} \tag{3.5}$$

so

$$H_0 = \frac{1}{2}\left(xp+px\right) = -i\hbar\sqrt{x}\frac{d}{dx}\sqrt{x} \tag{3.6}$$

This is a symmetric operator acting on a certain domain of the Hilert space $L^2(a,b)$, By definition, if an operator is symmetric (or Hermitian)[32]

$$\langle\psi|H_0\phi\rangle = \langle\psi H_0|\phi\rangle \tag{3.7}$$

or with limit,

$$\langle\psi|H_0\phi\rangle - \langle\psi H_0|\phi\rangle = i\hbar\left[a\psi^*(a)\phi(a) - b\phi^*(b)\psi(b)\right] = 0 \tag{3.8}$$

which is satisfied if both $\psi(x)$ and $\phi(x)$ vanish at the points a, b. von Neumann Theorem of deficiancy indices states that, an operator in symmetric if its deficiency indices $n_\pm$ are equal.[33]. Deficiency indices (or the defect numbers) of a closable symmetric operator T are cardinal number S

$$\begin{aligned} n_+ &:= d_\lambda = dim\ \mathcal{R}(T - \overline{\lambda}\mathbb{1})^\perp \quad Im\ \lambda > 0 \\ n_- &:= d_\lambda = dim\ \mathcal{R}(T - \overline{\lambda}\mathbb{1})^\perp \quad Im\ \lambda < 0 \end{aligned} \tag{3.9}$$

If T is densly defined and symmetric, then T is closable, and by formula $\mathcal{N}(T^*) = \mathcal{R}(T)^\perp$

$$\begin{aligned} n_+ &:= dim\ \mathcal{N}(T^* - i\mathbb{1}) = dim\ \mathcal{N}(T^* - \lambda\mathbb{1}) \quad Im\ \lambda > 0 \\ n_- &:= dim\ \mathcal{N}(T^* + i\mathbb{1}) = dim\ \mathcal{N}(T^* + \lambda\mathbb{1}) \quad Im\ \lambda < 0 \end{aligned} \tag{3.10}$$

By definition $n_\pm(T) = dim\ \mathcal{N}(T^* \mp iT)$

Again if T is a symmetric operator, then

$$\begin{aligned} K_+ &= ker\ (i\mathbb{1} - T^*) = Ran\ (i\mathbb{1} - T)^\perp \\ K_- &= ker\ (i\mathbb{1} + T^*) = Ran\ (-i\mathbb{1} + T)^\perp \end{aligned} \tag{3.11}$$

$K_+$ and $K_-$ are called the deficiency subspaces of T, The pair of numbers $n_+$, $n_-$ given by $n_+(T) = dim[K_+]$,$n_-(T) = dim[K_-]$ arre called deficiency indices of T.

von Neumann Theorem for deficiency indices states that if T an closed operator woth deficiency indices $n_+$ and $n_-$. Then

(1) T is symmetric if and only if $n_+ = n_- = 0$ ann self adjoint if $\mathcal{D}(T) = \mathcal{D}(T^*)$

(2) T is symmetric adn self adjoint and also has many self adjoint extensions if and only if $n_+ = n_- \neq 0$ and $\mathcal{D}(T) = \mathcal{D}(T^*)$. There is one-one correspondence between self adjoint extensions of T and unitary maps from $K_+$ onto $K_-$

(3) If either $n_+ = 0 \neq n_-$ or $n_- = 0 \neq n_+$ then T is not symmetric and has no nontrivial self adjoint extension (such operators are called maximal symmetric operator).

So this indices counts the number of solutions of the equation, which comes from the deficiency spaces for subsystem T

$$K_\pm = ker\left(-H_0^\dagger - \mp i\mathbb{1}\right) \tag{3.12}$$

which leads to find the solution of the equation.

$$H_0^\dagger \psi_\pm = \pm i\hbar\lambda\psi_\pm \tag{3.13}$$

belonging to the domain of $H_0^\dagger(\lambda > 0)$. If $n = n_+ = n_- > 0$, there are infinitely many self-adoint extensions of $H_0$ parameterized by a unitary $n \times n$ matrix. Stone's theorem states that if $U(t)$ be a strongly continuous one parameter unitary group on a Hilbert space $\mathcal{H}$. Then, there is a self-adjoint operator A on $\mathcal{H}$ so that $U(t) = e^{itA}$. The solution of the equation (3.13) is

$$
\begin{aligned}
H_0^\dagger \psi_\pm &= \pm i\hbar\lambda\psi_\pm \\
\implies H_0\psi_\pm &= \pm i\hbar\lambda\psi_\pm \qquad [because\ H_0\ is\ self-adjoint] \\
\implies \left(-i\hbar\sqrt{x}\frac{d}{dx}\sqrt{x}\right)\psi_\pm &= \pm i\hbar\lambda\psi_\pm \\
\implies -i\hbar\sqrt{x}\frac{d}{dx}\left(\sqrt{x}\psi_\pm\right) &= \pm i\hbar\lambda\psi_\pm \\
\implies -\sqrt{x}\frac{d}{dx}\left(\sqrt{x}\psi_\pm\right) &= \pm\lambda\psi_\pm \\
\implies -x\frac{d}{dx}\psi_\pm - \sqrt{x}\frac{1}{2\sqrt{x}}\frac{d}{dx}\psi_\pm &= \pm\lambda\psi_\pm \\
\implies -x\frac{d}{dx}\psi_\pm &= \left(\pm\lambda + \frac{1}{2}\right)\psi_\pm \\
\implies \frac{d}{dx}\psi_\pm &= -\frac{1}{x}\left(\pm\lambda + \frac{1}{2}\right)\psi_\pm \\
\implies \frac{d\psi_\pm}{\psi_\pm} &= -\frac{dx}{x}\left(\pm\lambda + \frac{1}{2}\right) \\
\implies ln\ \psi_\pm &= -\left(ln\ x\right)\left(\pm\lambda + \frac{1}{2}\right) + ln\ C \\
\implies \psi_\pm &= Cx^{-\frac{1}{2}\mp\lambda}
\end{aligned}
$$

whose norm in the interval (a,b) is

$$
\begin{aligned}
\langle\psi_\pm|\psi_\pm\rangle &= \int_a^b C^2 x^{-1\mp\lambda}\,dx \\
&= \mp\frac{C^2}{2\lambda}\left(b^{\mp 2\lambda} - a^{\mp 2\lambda}\right) \\
&= \pm\frac{C^2}{2\lambda}\left(a^{\mp 2\lambda} - b^{\mp 2\lambda}\right)
\end{aligned}
\tag{3.14}
$$

The deficiency indices correponding to the four intervals cosidered above are collecte in Table[34]. We find the deficency indices by observing different intervals. For BK intervals$(1, \infty)$ only $\psi_+$ belongs to Hilbert space ($\psi_-$ blows out. or putting intervals in Eq. (3.14) and testing whether it belongs to the Hilbert space)[31]. And the rest are given below

Table 3.1: Deficiency indices of $H_0$. The corresponding intervals are associated to the semiclassical regularizations of section 2 (BK, C ,S). The last one T, describes the case with no constraints on x except positivity (i.e. x>0)

| Type | (a,b) | $(n_+, n_-)$ | Self-adjoint |
|---|---|---|---|
| BK | $(1, \infty)$ | (1,0) | - |
| C | (0,N) | (0,1) | - |
| S | (1,N) | (1,1) | $\surd$ |
| T | $(0, \infty)$ | (0,0) | $\surd$ |

From the von Neumann theorem we see that $H_0$ is essentially self-adjoint on the half line $\mathbb{R}_+ = (0, \infty)$. This was studied by Twamley and Milbrn, who defined quantum Mellin transform using the eigenstates of $H_0$[35] On the other hand, in the interval (1,N) the operator $H_0$ admits infinitely many self-adjoint extensions parameterrized y a phase $e^{i\theta}$. This phase defines the boundary condition of the functions belonging to the self-adjoint domain.[31]

$$\mathcal{D}(H_{0,\theta}) = \left\{\psi, H_0\psi \in L^2(1, N), e^{i\theta}\psi(1) = \sqrt{N}\psi(N)\right\} \tag{3.15}$$

The eigenfunction of $H_0$

$$H_0\psi_E = E\psi_E, \tag{3.16}$$

are given by [12]

$$\psi_E(x) = \frac{C}{x^{\frac{1}{2}-iE\hbar}}, \qquad E \in \mathbb{R} \tag{3.17}$$

where C is a normalization constant. In the half line $\mathbb{R}_+$ there are no further restriction on E, hence the spectrum of $H_0$ is continuous and covers the whole real line $\mathbb{R}$. In this case the normalization constant is chosen as $C = \frac{1}{\sqrt{2\pi\hbar}}$ which gurantees the standard normalization

$$\langle\psi_E|\psi_{E'}\rangle = C^2\int_0^\infty \frac{dx}{x}x^{-i(E-E')/\hbar} = \delta(E-E') \tag{3.18}$$

In the case where $H_0$ is defined in ther interval, the boundary condition (3.13) yields the quantization condition for E, namely

$$\begin{aligned}
e^{i\theta}\psi(1) &= \sqrt{N}\psi(N) \\
\implies e^{i\theta}\frac{C}{1^{\frac{1}{2}-iE\hbar}} &= \sqrt{N}\frac{C}{N^{\frac{1}{2}-iE\hbar}} \\
\implies e^{i\theta} &= N^{-iE\hbar} \\
\implies i\theta &= (\frac{-iE}{\hbar})ln\ N \\
\implies E &= \frac{\hbar\theta}{ln\ N} \\
\implies E &= \frac{2\pi\hbar}{ln\ N}(\frac{\theta}{2\pi})
\end{aligned}$$

$$\implies E_n = \frac{2\pi\hbar}{ln\ N}(n + \frac{\theta}{2\pi}) \quad n \in \mathbb{N} \tag{3.19}$$

Hence the spectrum of $H_0$ is dscrete, with a level spacing decreasing for largerm values of N. The normalization constant of the wave function is now $C = \frac{1}{\sqrt{ln\ N}}$ which gives,

$$\langle \psi_{E_n} | \psi_{E_{n'}} \rangle = C^2 \int_1^N \frac{dx}{x} x^{-i(E_n - E_{n'})/\hbar} = \delta_{n,n'} \tag{3.20}$$

The spectrum (3.13) agrees with the semiclassical result given in Table 1 for the S-regularization(recall that $l_x = 1, \Lambda = N, \hbar = 1$) For the particular case where $\theta = \pi$, one observes that the energy spectrum is symmetric around zero, i.e, if $E_n$ is an eigenenergy so is $-E_n$. This result is obtained in working[36] with the inverse Hamiltonian $\frac{1}{H_0}$. We are reviewing that construction in next section.

## 3.2 The inverse Hamiltonain $1/H_0$

First, we take the expression at Eq(3.8) and take the formal inverse, i.e., $H_0^{-1} = x^{1/2}p^{-1}x^{1/2}$. The operator $p^{-1}$ is the one-dimensional Green's function with matrix elements(definition of Green's function: Green's function is the kernel of and integral operator that represents the inverse of a differential operator. Let

$$Lu = f \tag{3.21}$$

Here u and f are vectors and L is a square, invertible matrix. The inverse matrix exsits if $\lambda = 0$ is not an eigenvalue of L, or when det $detL \neq 0$. Now

$$u = L^{-1}f \tag{3.22}$$

where $L^{-1}$ is the inverse operator of L. The inverse operator to be an integral operator of the form.

$$\left(L^{-1}f\right)(x) = \int_a^b g(x,\xi)f(\xi)\,d\xi \tag{3.23}$$

with kernel G. If L exists, then the kernel fucntion $g(x,\xi)$ is called the Green's function associated with L.

So $p^{-1}$ operator will be

$$\begin{aligned}\left\langle x\middle|p^{-1}\middle|x^{'}\right\rangle &= \left\langle x\middle|\frac{1}{-i\hbar\frac{d}{dx}}\middle|x^{'}\right\rangle \\ &= -i\hbar\left\langle x\middle|\frac{1}{\frac{d}{dx}}\middle|x^{'}\right\rangle \\ &= \frac{\hbar}{i}G(x,x^{'}) \\ &= \frac{\hbar}{2i}sign(x-x^{'})\end{aligned} \tag{3.24}$$

Here $sign(x-x^{'})$ is the sign function.[36]. The operator $H_0^{-1}$ is defined in the interval (1,N) by the continuous matrix,

$$H_0^{-1}(x,x^{'}) = \frac{i}{2\hbar}\frac{sign(x-x^{'})}{\sqrt{xx^{'}}}, \quad 1 \leqslant x, x^{'} \leqslant N. \tag{3.25}$$

It's spectrum is found solving the Schrödinger equation.

$$\begin{aligned} & H_0(x,x^{'})\psi(x^{'}) = E\psi(x) \\ & \implies H_0^{-1}(x,x^{'})\psi(x^{'}) = E^{-1}\psi(x) \\ & \implies \frac{i}{2\hbar}\int_1^N dx^{'}\frac{sign(x-x^{'})}{\sqrt{xx^{'}}}\psi(x^{'}) = E^{-1}\psi(x) \end{aligned} \tag{3.26}$$

for the eigenvalue $E^{-1}$, which must not be singular for $H_0^{-1}$ to be invertible. Define a new wave function

$$\phi(x) = \frac{\psi(x)}{\sqrt{x}} \tag{3.27}$$

which satisfies

$$\frac{iE}{2\hbar}\int_1^N dx^{'} sign(x-x^{'})\phi(x^{'}) = x\phi(x) \tag{3.28}$$

Taking derivative with respect to x

$$\begin{aligned}
&\frac{d}{dx}\left(\frac{iE}{2\hbar}\int_1^N dx^{'} sign(x-x^{'})\phi(x^{'})\right) = \frac{d}{dx}\left(x\phi(x)\right) \\
&\implies \frac{iE}{2\hbar}\int_1^N dx^{'} 2\delta(x-x^{'})\phi(x^{'}) = \phi(x) + x\frac{d}{dx}\phi(x) \\
&\implies \frac{iE}{\hbar}\phi(x) = \phi(x) + x\frac{d}{dx}\phi(x) \\
&\implies x\frac{d}{dx}\phi(x) = \left(1-\frac{iE}{\hbar}\right)\phi(x) \qquad (3.29) \\
&\implies \frac{d\phi(x)}{\phi(x)} = \left(1-\frac{iE}{\hbar}\right)\frac{dx}{x} \\
&\implies ln\ \phi(x) = \left(1-\frac{iE}{\hbar}\right) ln\ x + ln\ C \\
&\implies \phi(x) = \frac{C}{x^{1-\frac{iE}{\hbar}}}
\end{aligned}$$

$$\psi(x) = \frac{C}{x^{1/2-\frac{iE}{\hbar}}} \qquad (3.30)$$

with $C = \frac{1}{\sqrt{ln\ N}}$ as in Eq(3.22). Eq(3.27) fixes the functional form of $\psi(x)$. To find the spectrum we impose (3.30) at one point , say $x = 1$, obtaining,

$$\begin{aligned}
&\frac{iE}{2\hbar}\int_1^N dx^{'} sign(1-x^{'})\phi(x^{'}) = \phi(1) \\
&\implies \frac{iE}{2\hbar}\int_1^N dx^{'} sign(1-x^{'})\frac{C}{x^{'1-iE/\hbar}} = \frac{C}{1^{1-iE/\hbar}} \qquad (3.31) \\
&\implies \frac{iE}{2\hbar}\int_1^N dx^{'} sign(1-x^{'})\frac{1}{x^{'1-iE/\hbar}} = 1
\end{aligned}$$

we know that sign function

$$sign(1-x^{'}) = \begin{cases} 1 & 1-x^{'} > 0 \implies 1 > x^{'} \\ 0 & 1-x^{'} = 0 \implies 1 = x^{'} \\ -1 & 1-x^{'} < 0 \implies 1 < x^{'} \end{cases}$$

Therefore

$$\frac{-iE}{2\hbar}\int_1^N dx^{'}x^{'-1+iE/\hbar} = 1$$
$$\frac{-iE}{2\hbar}\left[\frac{x^{'iE/\hbar}}{iE/\hbar}\right]_1^N = 1$$
$$\frac{1}{2}\left[N^{iE/\hbar} - 1^{iE/\hbar}\right] = 1$$
$$N^{iE/\hbar} - 1 = -2$$
$$N^{iE/\hbar} = -1$$
$$N^{iE/\hbar} = e^{i\pi}$$
$$\frac{iE}{\hbar} ln\ N = i\pi$$
$$E = \frac{\pi\hbar}{ln\ N}$$
$$E = \frac{2\pi\hbar}{ln\ N}\frac{1}{2}$$

$$\therefore E_n = \frac{2\pi\hbar}{ln\ N}\left[n + \frac{1}{2}\right] \tag{3.32}$$

This sprectrum coincides with (3.19) for $\theta = \pi$, so that the eigenstates come in pairs $\{E_n, -E_n\}$ as corresponds to an Hermitian antisymmetric operator. Including a BCS coupling , related to $\theta$ yields the spectrum (3.19)[35]

We take this spectrum and wavefunction to calculate OTOC(out of time order correlator)

# Chapter 4

# Out-of-Time-Order Correlator of Berry-Keating

First we formulate how to calculate the OTOC for generic quauntum mechanics. In particular, by the reason described above, we choose $W = x$ and $V = p$ to measure a possible indication of quantum chaos. We consider the out-of-time-order correlator (OTOC) defined by

$$C_T \equiv -\left\langle [x(t), p(0)]^2 \right\rangle \tag{4.1}$$

where $\langle \mathcal{O} \rangle \equiv \frac{tr\left[e^{-\beta H}\mathcal{O}\right]}{tr\ e^{-\beta H}}$. Here we define $\frac{1}{\beta}$ with the temperature of the system T. We will omit the argument of Heisenberg operators for $t = 0$; $\mathcal{O} \equiv \mathcal{O}(0)$. Taking energy eigenstates as the basis of the Hilber space, we can rewrite the OTOC as

$$C_T(t) = \frac{1}{Z}\sum_n e^{-\beta E_n} c_n(T) \tag{4.2}$$

$$c_n \equiv -\left\langle n\right|\left[x(t), p(0)\right]^2\left|n\right\rangle \tag{4.3}$$

where $H\left|n\right\rangle = E_n\left|n\right\rangle$. We will refer the OTOC for a fixed energy eigenstate, $c_n(t)$,as a microcanonical OTOC. On the other hand, we will refer $C_T(t)$ as a thermal OTOC. Once we compute microcanonical OTOCs, we can obtain the thermal OTOC bu taking their thermal average. Let us rewrite the microcanonical OTOC using matrix element of x and p for numerical calculations. Using the completeness relation $1 = \sum_m \left|m\right\rangle\left\langle m\right|$, we rewrite the microcanonical OTOC as

$$c_n(t) = \sum_m b_{nm}(t) b^*_{nm}(t) \tag{4.4}$$

$$b_{nm}(t) \equiv -i\left\langle n\right|\left[x(t), p(0)\right]\left|m\right\rangle \tag{4.5}$$

Note that $b_{nm}(t)$ is Hermitian: $b_{nm}(t) = b^*_{nm}(t)$. Substituting $x(t) = e^{iHt}xe^{-iHt}$ and inserting the completeness relation again, we obtain

$$
\begin{aligned}
b_{nm}(t) &= -i \left\langle n \right| \left[ e^{iHt} x e^{-iHt}, p \right] \left| m \right\rangle \\
&= -i \left\langle n \right| \left[ e^{iHt} x e^{-iHt} p - p e^{iHt} x e^{-iHt} \right] \left| m \right\rangle \\
&= -i \left[ \sum_k \left\langle n \right| e^{iHt} x e^{-iHt} \left| k \right\rangle \left\langle k \right| p \left| m \right\rangle - \sum_k \left\langle n \right| p \left| k \right\rangle \left\langle k \right| e^{iHt} x e^{-iHt} \left| m \right\rangle \right] \\
&= -i \left[ \sum_k \left\langle n \right| e^{iE_n t} x e^{-iE_k t} \left| k \right\rangle \left\langle k \right| p \left| m \right\rangle - \sum_k \left\langle n \right| p \left| k \right\rangle \left\langle k \right| e^{iE_k t} x e^{-iE_m t} \left| m \right\rangle \right] \\
&= -i \sum_k \left[ e^{iE_{nk} t} x_{nk} p_{km} - e^{iE_{km} t} p_{nk} x_{km} \right]
\end{aligned}
$$

$$
\therefore b_{nm}(t) = -i \sum_k \left[ e^{iE_{nk} t} x_{nk} p_{km} - e^{iE_{km} t} p_{nk} x_{km} \right] \tag{4.6}
$$

where $E = E_n - E_m$, $x_{nm} \equiv \langle n | \, x \, | m \rangle$ $p_{nm} \equiv \langle n | \, p \, | m \rangle$. In this expression, there are matrix components of p. They are not desirable since numerical derivatives of wave fuincitons lose the numerical accuracy. For a natural Hamiltonian with the form,

$$
H = \sum_{i=1}^{N} p_i^2 + U(x_1, \cdots, x_N) \tag{4.7}
$$

we can express $p_{nm}$using $x_{nm}$. We know from canonical commutation relation

$$[x, p] = i \qquad (\hbar = 1)$$

Therefore

$$\begin{aligned}
[H, x] &= [p^2 + U(x), x] \\
&= [p^2, x] + [U(x), x] \\
&= p[p, x] + [p, x]p \\
&= -ip - ip
\end{aligned}$$

$$\therefore [H, x] = -2ip \tag{4.8}$$

Applying $\langle m| \cdots |n\rangle$ to the both sides of the equation, we obtain

$$\begin{aligned}
&\langle m| [H, x] |n\rangle = \langle m| - 2ip |n\rangle \\
&\langle m| (Hx - xH) |n\rangle = -2i \langle m| p |n\rangle \\
&\langle m| (E_m x - x E_n) |n\rangle = -2ip_{mn} \\
&E_{mn} x_{mn} = -2ip_{mn} \\
&p_{mn} = \frac{i}{2} E_{mn} x_{mn}
\end{aligned}$$

Substituting this expression into (4.6) we have

$$b_{nm}(t) = \frac{-ii}{2}\sum_{k}(e^{iE_{nk}t}x_{nk}E_{km}x_{km} - e^{iE_{km}t}E_{nk}x_{nk}x_{km})$$

$$b_{nm}(t) = \frac{1}{2}\sum_{k} x_{nk}x_{km}(E_{km}e^{iE_{nk}t} - E_{nk}e^{iE_{km}t}) \tag{4.9}$$

Now we can take this equation to calculate OTOC of Berry-Keating Hamiltonian from (3.32). The spectrum is

$$E_n = \frac{2\pi\hbar}{ln\ N}\left[n + \frac{1}{2}\right] \tag{4.10}$$

and the wavefunction

$$\psi(x) = \frac{C}{x^{1/2-\frac{iE}{\hbar}}} \tag{4.11}$$

from here we can evaluate $x_{nm} = \langle n|\, x\, |m\rangle$ value

$$\begin{aligned}
\langle\psi_E|x|\psi_{E'}\rangle &= C^2\int_1^N \frac{dx}{x}x^{-i(E-E')/\hbar}x \\
&= C^2\int_1^N dx x^{-i(E-E')/\hbar} \\
&= C^2\left[\frac{x^{1-i(E-E')/\hbar}}{1-i(E-E')/\hbar}\right]_1^N \\
&= C^2\frac{1}{1-i(E-E')/\hbar}\left[N^{1-i(E-E')/\hbar}-1\right] \\
&= C^2\frac{1}{1-i(E-E')/\hbar}\left[N^{1-i(E-E')/\hbar}-1\right]
\end{aligned}$$

Therefore, $\langle n|\, x\, |m\rangle = x_{nm}$ is

$$\langle n|\, x\, |m\rangle = \frac{1}{ln\ N}\frac{1}{1-i\frac{2\pi\hbar}{\ln\ N}(n+\frac{1}{2}-m-\frac{1}{2})/\hbar}\left[N^{1-i\frac{2\pi\hbar}{\ln\ N}(n+\frac{1}{2}-m-\frac{1}{2})/\hbar}-1\right] \tag{4.12}$$

$$x_{nm} = \frac{1}{ln\ N}\frac{1}{1-i\frac{2\pi}{\ln\ N}(n+\frac{1}{2}-m-\frac{1}{2})}\left[N^{1-i\frac{2\pi}{\ln\ N}(n+\frac{1}{2}-m-\frac{1}{2})}-1\right] \tag{4.13}$$

putting these values on Eq(4.9)

$$b_{nm}(t) = \frac{1}{2}\sum_k x_{nk}x_{km}(E_{km}e^{iE_{nk}t} - E_{nk}e^{iE_{km}t})$$

and calculate OTOC analytically. cause carry out the summation of $x_{nm}$ and energy eigenstates makes things little complicated. The graph and codes are given below.

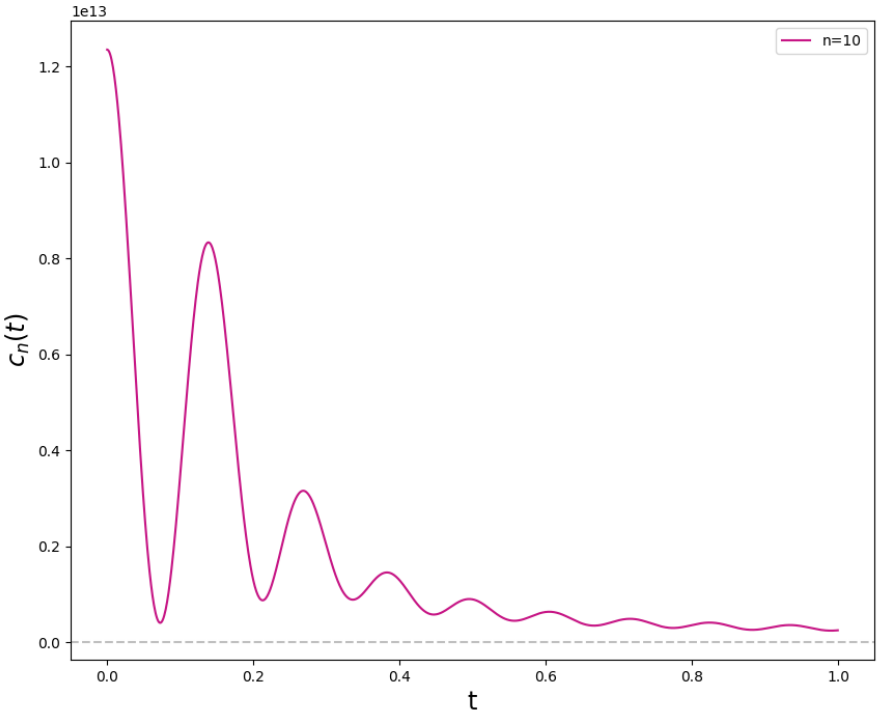


Figure 4.1

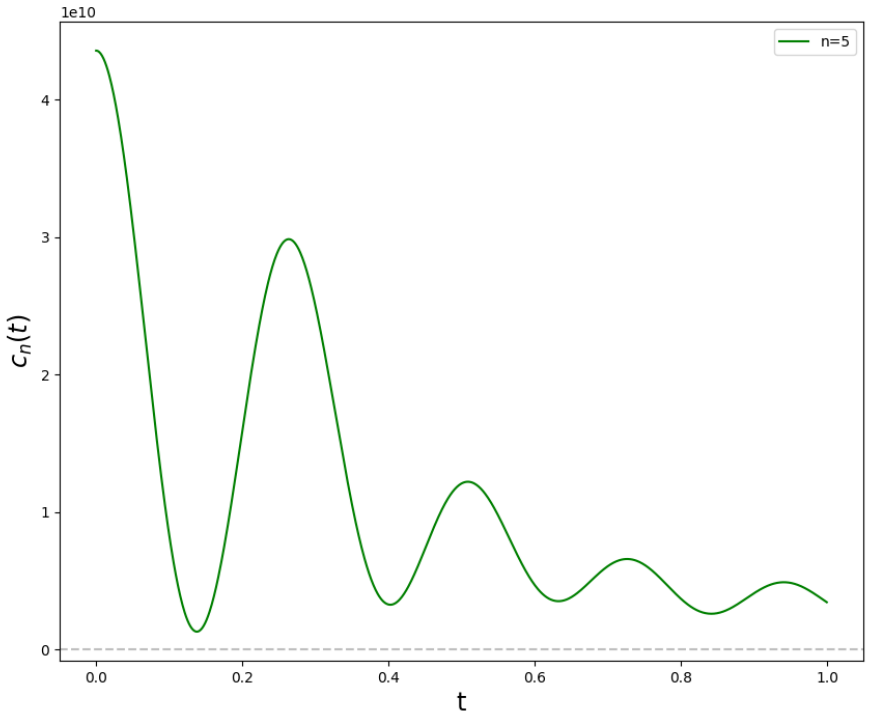


Figure 4.2
Here microcanonical OTOC and thermal OTOC are same with different temperatures.

```
import numpy as np
import matplotlib.pyplot as plt
import math
import cmath

a = [] #initialize some list to plot data
b = []
r=6    # matrix dimension number
```

```
N=10    #Higest interval in the spectrum
T=40    #temperature


#function for spetrum E_{nm}
def E(n, m):
    return (2*math.pi*(n-m))/(math.log(N))


#function for position x_{nm}
def x(n, m):
    a = (1/1-(2j*math.pi*(n-m)/math.log(N)))/(math.sqrt(math.
   log(N)))
    b = (N**(1-(2j*math.pi*(n-m)/math.log(N)))-1)
    return a*b


#calculating Thermal OTOC C_{T}
for t in np.arange(0,1,0.001):
    Z=0
    C=0
    s3=0

    for n in range(0,r):
        s2 = 0

        for m in range(0,r):
```

```
35              s1=0
36
37              for k in range(0,r):
38                  s1 += (1/2.0)*x(n,k)*x(k,m)*(E(k,m)*cmath.exp
    (1j*E(n,k)*t) - E(n,k)*cmath.exp(1j*E(k,m)*t))
39
40              s2 += s1*np.conjugate(s1)
41
42     #partition function
43     Z += cmath.exp(-E(n,0)/T)
44
45     #e^{-\beta E_n} O
46     C += (cmath.exp(-E(n,0)/T)*s2)
47
48     #expectation value or Thermal OTOC
49     s3=C/Z
50
51
52     a.append(t)
53     b.append(s3)
54
55
56 #for plot
57 f = plt.figure()
58 f.set_figwidth(10)
59 f.set_figheight(8)
60 plt.plot(a, b, label='n=10', color='mediumvioletred')
```

```
plt.ylabel('$c_{n}(t)$',fontsize=30)
plt.xlabel('t',fontsize=30)
plt.legend()
plt.show()



f = plt.figure()
f.set_figwidth(10)
f.set_figheight(8)
plt.plot(a, b, label='n=5', color='green')
plt.ylabel('$c_{n}(t)$',fontsize=30)
plt.xlabel('t',fontsize=40)
plt.axhline(0,ls='--',alpha=0.5,c='grey')
plt.legend()
plt.savefig('test.png')
```

Listing 4.1: Python example

We also used Markov Chain Monte Carlo Method/Hamiltonian Monte Carlo Method [37, 38] and obtained same result. The graph and codes are given below.

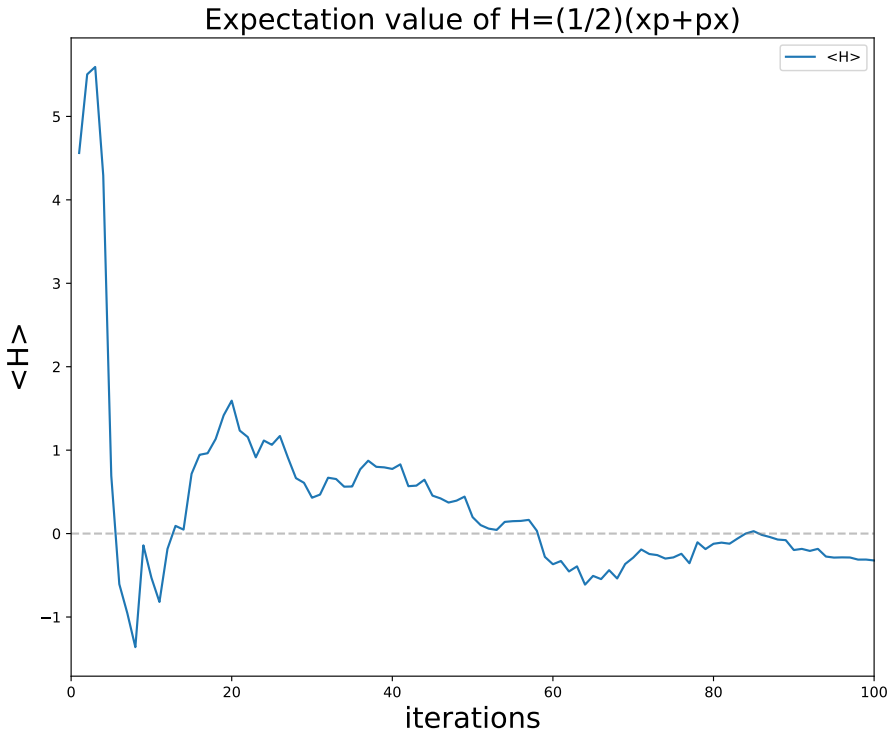


Figure 4.3

```
#ifndef MATRIX
#define MATRIX


#include<complex>
using namespace std;

//matrix dimension
const int n=10;

```

```
11
12 /*
13     Declaring a function for easily calling a matrix, it 2nd,
       3rd, 4th order terms, and their traces.
14 */
15 double matrix(complex<double> A[n][n], complex<double> (&A2)[
       n][n], complex<double> (&A3)[n][n], complex<double> (&A4)[
       n][n], double& s, double& s2, double& s3, double& s4)
16 {
17     s=0, s2=0, s3=0, s4=0;
18
19     // 2nd Order matrix
20     for(int i=0; i<n; i+=1)
21     {
22         for(int j=0; j<n; j+=1)
23         {
24             for(int k=0; k<n; k+=1)
25             {
26                 A2[i][j] += A[i][k]*A[k][j];
27             }
28         }
29     }
30
31     //  3rd order matrix
32     for(int i=0; i<n; i+=1)
33     {
34         for(int j=0; j<n; j+=1)
```

```
35          {
36              for(int k=0; k<n; k+=1)
37              {
38                  A3[i][j] += A2[i][k]*A[k][j];
39              }
40          }
41      }
42
43      // 4th order matrix
44      for(int i=0; i<n; i+=1)
45      {
46          for(int j=0; j<n; j+=1)
47          {
48              for(int k=0; k<n; k+=1)
49              {
50                  A4[i][j] += A3[i][k]*A[k][j];
51              }
52          }
53      }
54
55      //  Trace of A
56      for(int i=0; i<n; i+=1)
57      {
58          s += A[i][i].real();
59      }
60
61      // Trace of A^2
```

```
62      for(int i=0; i<n; i+=1)
63      {
64          s2 += A2[i][i].real();
65      }
66
67      //  Trace of A^3
68      for(int i=0; i<n; i+=1)
69      {
70          s3 += A3[i][i].real();
71      }
72
73      //  Trace of A^4
74      for(int i=0; i<n; i+=1)
75      {
76          s4 += A4[i][i].real();
77      }
78
79      return 0;
80  }
81
82  #endif
```

Listing 4.2: matrix.h

```
1  #ifndef BOX
2  #define BOX
3
4
```

```
5  #include<cstdlib>
6  #include<cmath>
7  #include<random>
8  using namespace std;
9
10
11 //Gaussian Random Number Generator with Box Muller Algorithm
12 double Box(double& x, double& y)
13 {
14     //uniform random numbers between 0 and 1
15     random_device rd;
16     mt19937 mt(rd());
17     uniform_real_distribution<double> r1(0, 1);
18     double p,q;
19
20     p = r1(mt);
21     q = r1(mt);
22
23
24     //Gaussina random numbers with weights proportional to e
       ^{-x^2/2} and e^{-y^2/2}
25     x = sqrt(-2*log(p))*sin(2*M_PI*q);
26     y = sqrt(-2*log(p))*cos(2*M_PI*q);
27
28
29     return 0;
30 }
```

```
31
32 #endif
```

Listing 4.3: box.h

```
1  #ifndef HAM
2  #define HAM
3
4
5
6  /*
7      Calculating Hamiltonian of Berry-Keating H = (1/2)(xp+px)
8  */
9  double hamiltonian(complex<double> A[n][n], complex<double> B
       [n][n])
10 {
11
12     // A is a matrix of x
13     //B is a matrix of p
14     complex <double> H[n][n] = {0}, N1[n][n] = {0}, N2[n][n]
       = {0};
15     double sum=0;
16
17
18     for(int i=0; i<n; i+=1)
19     {
20         for(int j=0; j<n; j+=1)
21         {
```

```
22              for(int k=0; k<n; k+=1)
23              {
24                  // x*p
25                  N1[i][j] += A[i][k]*B[k][j];
26              }
27          }
28      }
29
30
31      for(int i=0; i<n; i+=1)
32      {
33          for(int j=0; j<n; j+=1)
34          {
35              for(int k=0; k<n; k+=1)
36              {
37                  // p*x
38                  N2[i][j] += B[i][k]*A[k][j];
39              }
40          }
41      }
42
43
44      for(int i=0; i<n; i+=1)
45      {
46          for(int j=0; j<n; j+=1)
47          {
48              // xp + px
```

```
49              H[i][j] = N1[i][j] + N2[i][j];
50          }
51      }
52
53
54      for(int i=0; i<n; i+=1)
55      {
56          sum += H[i][i].real();
57      }
58
59
60      return 0.5*sum;
61  }
62
63
64  #endif
```

Listing 4.4: hamiltonian.h

```
1  #ifndef FORCE
2  #define FORCE
3
4  #include<~/matrix.h>
5
6
7  /*
8      Calculating force (dH/d phi = dS/d phi) term = p
9  */
```

```
10
11 double force(complex<double> A[n][n], complex<double> (&dh)[n
       ][n])
12 {
13     // calculating force matrix
14     for(int i=0; i<n; i+=1)
15     {
16         for(int j=0; j<n; j+=1)
17         {
18             // dh = dH/dphi
19             dh[i][j] = (A[i][j]);
20         }
21     }
22
23     return 0;
24 }
25
26 #endif
```

Listing 4.5: force.h

```
1 #ifndef MOL
2 #define MOL
3
4 #include<~/box.h>
5 #include<~/force.h>
6 #include<~/hamiltonian.h>
7
```

```
8
9
10 /*
11     Molecular dynamics part
12 */
13 double molecular(complex<double> (&phi)[n][n], complex<double
       > (&P)[n][n], double& hi, double& hf)
14 {
15
16     double p, q, r1, r2,nt=10;
17
18     complex<double>  dt=0.001, dh[n][n] = {0};
19
20     for(int i=0; i<n; i+=1)
21     {
22         for(int j=0; j<n; j+=1)
23         {
24             Box(p,q);
25             P[i][j] = complex(p/sqrt(2),q/sqrt(2));
26         }
27     }
28
29     // Initial hamiltonian of molecular dynamics
30     hi = hamiltonian(phi,P);
31
32
33     //leap frog method
```

```
34      // xi(dt/2) = xi(0) + pi(0)dt/2;
35      for(int i=0; i<n; i+=1)
36      {
37          for(int j=0; j<n; j+=1)
38          {
39              phi[i][j] += 0.5*P[i][j]*dt;
40          }
41      }
42
43      // for n=1 to nt steps
44      //pi(ndt) = pi((n-1)dt) - (ds/dx)((n-1/2)dt)dt
45      for(int i=1; i<=nt-1; i+=1)
46      {
47          //calling force term
48          force(P,dh);
49          for(int j=0; j<n; j+=1)
50          {
51              for(int k=0; k<n; k+=1)
52              {
53                  P[j][k] -= dh[j][k]*dt;
54                  phi[j][k] += P[j][k]*dt;
55              }
56          }
57      }
58
59      //calling force term
60      //late step of leap frog method
```

```
61      //pi(nt *dt) = pi((nt-1)dt) -  (ds/dx)((nt-1/2)dt)dt
62      //xi(nt* dt) = xi((nt-1)dt) + p(nt *dt) dt/2;
63      force(P,dh);
64      for(int i=0; i<n; i+=1)
65      {
66          for(int j=0; j<n; j+=1)
67          {
68              P[i][j] -= dh[i][j]*dt;
69              phi[i][j] += 0.5*P[i][j]*dt;
70          }
71      }
72
73      //final hamiltonian of molecular dynamics
74      hf = hamiltonian(phi,P);
75
76      return 0;
77  }
78
79  #endif
```

Listing 4.6: molecular.h

```
1  #include<~/box.h>
2  #include<~/force.h>
3  #include<~/molecular.h>
4  #include<~/matrix.h>
5  #include<iostream>
6  #include<cmath>
```

```
7  #include<fstream>
8  #include<cstdlib>
9  #include<complex>
10 #include<ctime>
11 #include<random>
12 using namespace std;
13
14 double fact(double x)
15 {
16     double s=1;
17     for(int i=1; i<=x; i+=1)
18     {
19         s *= i*(i+1);
20     }
21
22     return s;
23 }
24
25 int main()
26 {
27     srand(time(NULL));
28     ofstream fout("main.dat");
29     ofstream file("part.dat");
30     double hi, hf, s=0, s2=0, r,
31     c=0,p,q,C[10000]={},x=0,a=0, D[10000][10]={};
32     long double x1=0, x2, y1=0, y2=0;
33     const int n=10;
```

```
34      double t = 198;
35      //x=0;
36      complex<double> A[n][n] = {0},
37      A0[n][n] = {0},B[n][n] = {0},B0[n][n] = {0};
38
39          //generating random value for x
40          for(int i=0; i<n; i+=1)
41          {
42              for(int j=0; j<n; j+=1)
43              {
44                  p=(double)rand()/(double)RAND_MAX;
45                  q=(double)rand()/(double)RAND_MAX;
46                  A[i][j]=complex(p,q);
47              }
48          }
49
50          //metropolis test
51          for(int i=1; i<10000; i+=1)
52          {
53              for(int j=0; j<n; j+=1)
54              {
55                  for(int k=0; k<n; k+=1)
56                  {
57                      //x0=x
58                      A0[j][k] = A[j][k];
59
60                  }
```

```
61              }
62
63              molecular(A,B,hi,hf);
64              r = (double)rand()/(double)RAND_MAX;
65              if(exp(hi-hf)>r)
66              {
67                  c+=1;
68              }
69
70              else
71              {
72                  for(int j=0; j<n; j+=1)
73                  {
74                      for(int k=0; k<n; k+=1)
75                      {
76                          A[j][k] = A0[j][k];
77                      }
78                  }
79              }
80
81              s = hamiltonian(A,B);
82              s2 += hamiltonian(A,B);
83              C[i] = s;
84              fout << i << "  " << (double)s/(double)i
85              << "  " << (double)s2/(double)(i) << endl;
86          }
87
```

```
88          //calculating partition function
89          y1=0, x1=0;
90          for(int i=1; i<10000; i+=1)
91          {
92              y1 += exp(-C[i]/t);
93
94          }
95
96          // sum of <H>*exp(-\beta H)/Z
97          for(int i=1; i<10000; i+=1)
98          {
99              x1 += C[i]*exp(-C[i]/t);
100
101             file << i << "  " << x1/y1 << endl;
102
103         }
104
105
106
107     return 0;
108 }
```

Listing 4.7: main.cpp

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3
4 a = np.loadtxt("main.dat")
```

```
5
6  f = plt.figure()
7  f.set_figwidth(10)
8  f.set_figheight(8)
9  plt.plot(a[:,0], a[:,2], label='<H>')
10 plt.xlim([0,100])
11 plt.axhline(0, c='grey', alpha=0.5, ls='--')
12 plt.xlabel("iterations", fontsize=20)
13 plt.ylabel("<H>", fontsize=20)
14 plt.title("Expectation value of H=(1/2)(xp+px)", fontsize=20)
15 plt.legend()
16 plt.show()
17
18
19 f = plt.figure()
20 f.set_figwidth(10)
21 f.set_figheight(8)
22 plt.plot(a[:,0], a[:,2], label='<H>')
23 plt.xlim([0,100])
24 plt.axhline(0, c='grey', alpha=0.5, ls='--')
25 plt.xlabel("iterations", fontsize=20)
26 plt.ylabel("<H>", fontsize=20)
27 plt.title("Expectation value of H=(1/2)(xp+px)", fontsize=20)
28 plt.legend()
29 plt.savefig("plot.pdf")
```

Listing 4.8: plot.py

# Chapter 5

# Conclusions

In this paper, we discussed what is Riemann hypothesis is, and why it is important to the field to quantum mechanics. The imaginary part of Hamiltonian proposed by Berry-Keating Hamiltonian $H_0 = \frac{1}{2}(xp+px)$ shows the self-adjoint and quanutm chaos. We look at Sierra regularization of Berry-Keating Hamiltonian, and their intervals $l_x = 1, \Lambda = 1$ and evaluated the spectrum $E_n = \frac{2\pi\hbar}{ln\ N}(n + \frac{\theta}{2\pi})$ of $\psi_E(x) = \frac{C}{x^{\frac{1}{2}-iE\hbar}}$ eigenfunction. Then we look at the quantization of inverse Hamiltonian $H_0^{-1} = x^{-1/2}p^{-1}x^{1/2}$ and obtained the spectrum $E_n = \frac{2\pi\hbar}{ln\ N}(n+\frac{1}{2})$ which is reckon to be $E_n = \frac{2\pi\hbar}{ln\ N}(n+\frac{\theta}{2\pi})$ with $\theta = \pi$

We discussed OTOC in quantum mehcanics and it thermal and microcanonical relation between them. We input the spccetrum and position operator of inverse Hamiltonaian and calculate its quantum chaos analytically. We see that microcanonical OTOC settles at value greater than zero while

the thermal OTOC displays the same behaviour of microcanonical OTOC.

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