AN EXORDIUM TO QUANTUM FIELD THEORY AND A BRIEF STUDY OF CHAOTIC SYSTEMS AND ITS DETERMINATION

M.Sc. Project Report

submitted in partial fulfillment of the requirement for the degree of

MASTER IN SCIENCE, PHYSICS

by

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DECLARATION

I hereby declare that the report of the project work entitled "AN EXORDIUM TO QUANTUM FIELD THEORY AND A BRIEF STUDY OF CHAOTIC SYSTEMS AND ITS DETERMINATION" which is submitted to National Institute of Technology Karnataka, Surathkal, in partial fulfillment of the requirement for the award of the Degree of Master of Science in the Department of Physics, is a bonafide report of the work carried out by me. The material contained in this report has not been submitted to any University or Institution for the awards of any degree.

Place: Surathkal

Date: 10 August 2021

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CERTIFICATE

This is to certify that the project entitled "AN EXORDIUM TO QUANTUM FIELD THEORY AND A BRIEF STUDY OF CHAOTIC SYSTEMS AND ITS DETERMINATION" is an authenticated record of work carried out by SHREYA PANDEY, Roll No.: 196PH019 in partial fulfillment of the requirement for the award of the Degree of Master of Science in Physics which is submitted to Department of Physics, National Institute of Technology Karnataka, Surathkal, during the period 2020-2021.

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ABSTRACT

This project report discusses about the detailed evolution of Quantum Field Theory. Putting forward the limitations of Quantum Mechanics, it motivates the importance of Field approach in various on-going experiments. It starts from Klein Gordon Equation, the first relativistic wave equation describing bosons, moving ahead to Dirac Equation which describes Fermions and then discussing the significance of building field theory.

The out-of-time-order correlator (OTOC) is considered as a measure of quantum chaos. We formulate steps for calculating the OTOC for quantum mechanics with a general Hamiltonian. We demonstrate calculations of OTOCs by taking an example of a 1D harmonic oscillator as it forms a fundamental basis for any quantum field theory. This OTOC is found to be periodic in time because of its commensurable energy spectra. We also look at a system with two non linearly coupled harmonic oscillators and see the exponential growth of its thermal OTOC.

OBJECTIVES

The objective of this project is to build a theory which is the most fundamental of all and which can give the deterministic description of reality. For building such a theory, it is required to make it relativistically invariant, that is, its laws doesn't change for different observers moving at different speeds. The limitations in making relativistically invariant version of Quantum Mechanics lead us to take **field** approach. It is also required for such a theory to be **Causal**. The Field approach lead us to describe various interactions taking place in complicated systems and also explains the existence of **antiparticles**. These interactions can be represented using **Feynman Diagrams**.

We also aim to build an understanding of Chaotic Systems and how they are measured in classical and quantum realm. For measuring classical chaos, we use the Lyapunov Exponents and Poincare surfaces of section whereas, Out-Of-Time-Ordered-Correlators(OTOC) is an indicator of Quantum Chaos.

We consider a system of two harmonic oscillators coupled nonlinearly with each other, and numerically observe that the thermal OTOC grows exponentially in time.

LITERATURE REVIEW

Quantum field theory naturally began with the study of electromagnetic interactions, as the electromagnetic field was the only known classical field as of the 1920s. It was first created by Paul Dirac when he attempted to quantize electromagnetic fields. The later advancement in this field led to the introduction of Quantum Electrodynamics. This theory became so successful that it could accurately predict and explain the standard models in particle physics and condensed matter physics. Quantum Field theory has important application in calculating on shell scattering amplitudes which was published in 2014 by Henriette Elvang, Yu-tin Huang [3].

In this report, the development of Quantum Field theory has been discussed so far. In order to study about how this theory evolved, I referred to Ashok Das's Lecture notes on Quantum field Theory [2] which has a very detailed and deep insight of the subject . I also referred to the book by Tom Lancaster, Stephen J. Blundell, named Quantum Field Theory for the Gifted Amateur [5], which was published in 2014. This book has a very descriptive and interesting way of explaining the concepts with some perfect set of examples. The most standard writings in this field is by Michael E. Peskin, Daniel V. Schroeder, An Introduction to Quantum Field Theory, published in 1995 [8] which incorporates all the necessary concepts in a compact way. I also followed lectures notes by David Tong [10] for mathematical derivations.

Quantum field theory can be applied to various Chaotic Systems. A recent paper on OTOC in couple harmonic oscillators by Tetsuya Akutagawa, Koji Hashimoto, Toshiaki Sasaki, Ryota Watanabe was published in 2020 [1]. It explains how OTOC act as an indicator of Quantum Chaos.I reviewed this paper in my project work. I have also taken assitance from an article on Out-Of-Time-Ordered Correlators in Quantum mechanics for all the analytical calculation for computation of OTOC.[4] I did further reading on the various applications of chaos in high energy physics from [6, 7]. At the end, I referred to Quantum mechanical out-of-time-ordered-correlators for the anharmonic (quartic) oscillator by Paul Romatschke published most recent in 2021[9] for studying its chaotic behavior.

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III semester: Introduction

The Aim of this project is to understand the basic concepts of Quantum Field Theory. It has a brief discussion on the limitations of Quantum Mechanics and the need for the fields. We start with finding a relativistic equation which must be Invariant under various transformations. We require our theory to be causal in order to define a physical system. The limitations of Schrodinger equation led to Klein Gordon equation, the inconsistencies of which were further resolved by Paul Dirac in Dirac Equation. In order to make our theory a multiparticle theory, We introduced the concept of field variable which can be described for infinite degrees of freedom. We started by writing the hamiltonian of such field and then doing canonical quantization in order to obtain the dynamical equation of motion for the particle in such fields. It was found that the solution of these equations lead us to consider our field equations as linear superposition of simple harmonic oscillators which can be easily quantized to give infinite number of oscillators. After quantization, the field variable is treated as operators. In order to calculate the amplitudes of various interaction processes, We then introduce a quantity called Propagator which measures the amplitude of particle going from one position to other in spacetime and with the help of this quantity, We calculate the amplitude of various Scattering Experiments which involves interactions.

1 Need Of Fields

1.1 Limitation of Schrodinger's Equation

The time dependent schrodinger equation is given as:

$$\iota\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi \tag{1}$$

This equation is linear in the time derivative while it is quadratic in the space derivatives. Therefore, space and time are not treated on an equal footing in this case and, consequently, the equation cannot be Lorentz invariant. Our requirement is that A relativistic equation must treat space and time coordinates on an equal footing and remain form invariant in all inertial frames (Lorentz Invariant). Thus this equation does not apply in relativistic cases.

1.2 The death of single-particle quantum mechanics

If We want to find 'what is the amplitude for a particle to travel outside its forward light-cone?' or in other words: 'what is the amplitude for a particle at the spacetime origin(x = 0, t = 0) to travel to position x in time t which would require it to travel faster than light making the interval spacelike?' If this amplitude is found to be non-zero then, the probability of particle to travel outside the forward light cone is also non zero which is unacceptable and would spell the death of quantum theory.[5] Calculating this amplitude

$$A =< x|e^{-\iota\hat{H}t}|x = 0 > \tag{2}$$

We find that this amplitude is non-zero and is given by $e^{-m|\mathbf{x}|}$. Therefore, Reconciliation of special relativity with single particle quantum mechanics is not possible and thus we have to switch to **Field theory**.

2 Quantum Field Theory

In QFT, Every particle or wave is considered to be an excitation of field defined over all space and time. It describes interaction of complicated systems.

2.1 What are Fields

Field is an entity that gives "amplitude of something" at each point in spacetime and the amplitude can be vector, scalar, tensor or tensors.

3 Notation and Basic Definition

3.1 Euclidean space

It is a 3 Dimensional space. A Vector in Euclidean space is defined as

$$\mathbf{A} = (A_1, A_2, A_3) \tag{3}$$

In Euclidean space, Scalar product of two arbitrary vectors A and B is defined as

$$\mathbf{A}.\mathbf{B} = A_i B_i = \delta_{ij} A_i B_j \tag{4}$$

Length of a vector is given as

$$\mathbf{A^2} = \mathbf{A}.\mathbf{A} = A_i A_i = \delta_{ij} A_i A_j \tag{5}$$

The length of the vector need to be positive always ,thus,

$$\boxed{\mathbf{A^2} \geq 0} \tag{6}$$

3.2 Minkowski Space

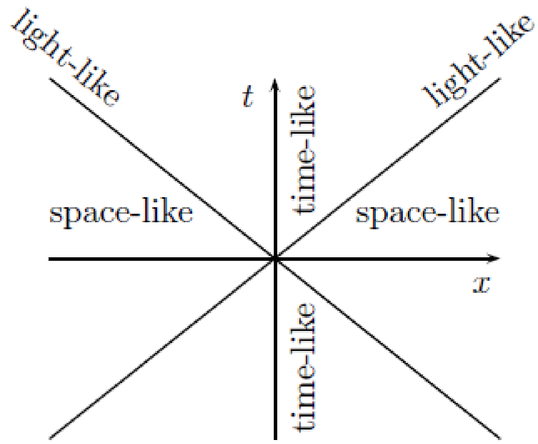


Figure 1: Different invariant regions of Minkowski space.

Enlarging the three Dimensional Euclidean manifold into four Dimensional spacetime manifold and by treating space and time on equal footing, we define a space where every vector has four components and is known as Four vector.

Four Vectors: Four vector has 1 timelike and 3 spacelike components.They are two following types:-

Contravariant Vector: Taking c=1,

$$x^{\mu} = (t, \mathbf{x}) \tag{7}$$

Covariant Vector:

$$x_{\mu} = (t, -\mathbf{x}) \tag{8}$$

They have distinct transformation properties under Lorentz transformation and transform inversely to each other.

They are related to each other by a metric tensor in Minkowski Space as:

$$x^\mu = \eta^{\mu\nu} x_\nu \tag{9}$$

$$x_\mu = \eta_{\mu\nu} x^\nu \tag{10}$$

$$\eta^{\mu\lambda}\eta_{\lambda\nu} = \delta^\mu_\nu \tag{11}$$

Scalar product in Minkowski Space is defined as:-

$$A.B = A^\mu B_\mu = A_\mu B^\mu \tag{12}$$

$$\boxed{A.B = A^0 B^0 - \mathbf{A}.\mathbf{B}} \tag{13}$$

Unlike Euclidean Space, length of vector need not be always positive in Minkowski Space. So,

$$x^2 = x^\mu x_\mu = t^2 - \mathbf{x^2} \tag{14}$$

If

$$x^2 = t^2 - \mathbf{x^2} > 0, \tag{15}$$

then **timelike** space
If

$$x^2 = t^2 - \mathbf{x^2} < 0, \tag{16}$$

then **spacelike** space

- **Contragradient**

$$\partial^\mu = \frac{\partial}{\partial x_\mu} = (\frac{\partial}{\partial t}, -\nabla) \tag{17}$$

- **Cogradient**

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = (\frac{\partial}{\partial t}, \nabla) \tag{18}$$

Also , Defining a Lorentz invariant quantity called De'Alembertain:-

$$\boxed{\Box = \partial^2 = \partial^\mu \partial_\mu = (\frac{\partial^2}{\partial t^2}, -\nabla^2)} \tag{19}$$

Now, Defining energy-momentum four vector as:-

$$p^\mu = (E, \mathbf{p}) \tag{20}$$

$$p^\mu = i\hbar\partial^\mu = i\hbar\frac{\partial}{\partial x_\mu} = (i\hbar\frac{\partial}{\partial t}, -i\hbar\nabla) \tag{21}$$

$$p_\mu = (E, -\mathbf{p}) \tag{22}$$

$$p_\mu = i\hbar\partial_\mu = i\hbar\frac{\partial}{\partial x^\mu} = (i\hbar\frac{\partial}{\partial t}, i\hbar\nabla) \tag{23}$$

Also,

$$p^2 = p^\mu p_\mu = E^2 - \mathbf{p^2} \tag{24}$$

From Einstein's Relation:

$$E^2 = \mathbf{p^2} + m^2 \tag{25}$$

From eq(24) and eq.(25)

$$p^2 = m^2 = E^2 - \mathbf{p^2} \tag{26}$$

Energy and momentum of a free particle must be lying on the hyperbola satisfying above equation.

4 Klein Gordon equation

We know that Schrodinger Equation is not Lorentz Invariant because of being second order in space derivatives and first order in time derivatives which makes it inconsistent with special relativity. Thus, The limitations of Schrodinger Equation leads to forming an equation that treats space and time on equal footing so as to make it consistent with special relativity. So, Klein Gordon Equation is such a relativistic wave equation which describes a single free particle without any spin.[2] The key-points about Klein Gordon Equation are:

- It is a relativistic wave equation like Schrodinger wave equation.
- Unlike Schrodinger Equation, It is second order in both space and time.
- It is Lorentz Invariant.
- Like wave equation, Klein Gordon equation also has plane wave solution (characteristic of free particle)

In non-relativistic case, Energy-momentum relation is given as:-

$$E = \frac{\mathbf{p^2}}{2m} + V(x) \tag{27}$$

In Relativistic case, Energy-momentum relation is given by Einstein relation as in eq.(25).
We know,

$$p^2 = p^\mu p_\mu = m^2 = E^2 - \mathbf{p^2} \tag{28}$$

Applying p^2 on a scalar function ϕ, we get,

$$(p^\mu p_\mu)\phi = m^2\phi \tag{29}$$

$$(i\hbar\partial^\mu)(i\hbar\partial_\mu)\phi = m^2\phi \tag{30}$$

$$(-\hbar^2\partial^\mu\partial_\mu)\phi = m^2\phi \tag{31}$$

Putting $\hbar = 1$,

$$\boxed{(\Box + m^2)\phi = 0} \tag{32}$$

This is the Klein Gordon equation in which ∂^2 and m^2 both are lorentz scalar thus making eq.(32) Lorentz invariant.

4.1 Solution of Klein Gordon Equation

Considering the scalar function $\phi = \phi(x, t)$ For m=0, writing eq.(33) :

$$\partial^2\phi = 0 \tag{33}$$

$$(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2})\phi = 0 \tag{34}$$

Above equation is similar to the wave equation:

$$(\frac{\partial^2}{\partial t^2} - \nabla^2)\phi = 0 \tag{35}$$

Thus the solution of Klein Gordon equation is plane wave solution represented as:

$$\phi = \exp\{(\mp k.x)\} \tag{36}$$

Putting this solution back in eq.(33), we get the relation,

$$(k^2 + m^2)\phi = 0 \tag{37}$$

$$(-(k^0)^2 + \mathbf{k^2} + m^2) = 0 \tag{38}$$

$$k^0 = \pm\sqrt{\mathbf{k^2} + m^2} = \pm E(energy) \tag{39}$$

Above relation shows that if eq.(39) is satisfied by k^0 , then the solution of ϕ will be same for m=0 and $m \neq 0$.

4.2 Problem with Klein Gordon Equation

The relation in eq.(39) gives both positive and negative energy solutions which is inconsistent with the probability density theory Writing the Klein Gordon Equation and its complex conjugate,

$$(\partial^2 + m^2)\phi = 0 \tag{40}$$

$$(\partial^2 + m^2)\phi^* = 0 \tag{41}$$

Multiplying eq.(40) by ϕ^* and eq.(41) by ϕ and subtracting , we get:

$$\boxed{\frac{\partial \rho}{\partial t} - \nabla . J = 0} \tag{42}$$

$$where : \rho = (\phi^* \frac{\partial \phi}{\partial t} - \phi \frac{\partial \phi^*}{\partial t}) \tag{43}$$

$$J = (\phi^* \nabla \phi - \phi \nabla \phi^*) \tag{44}$$

Eq.(42) is the continuity equation. Now, Putting the value of ϕ from eq.(36) in eq.(43), we get:

$$\boxed{\rho = \frac{k^0}{m} = \frac{\pm E}{m}} \tag{45}$$

Thus, the problem of negative energy shows up.

4.3 Limitations of Klein Gordon Equation

- It gives both positive and negative energy solution. We can't ignore negative energy states as positive states won't form complete basis in Hilbert space.
- It is second order in time derivative which is the reason for probability density being first order in time derivative and hence, showing up negative energy states problem.

Thus, the conclusion is that in order to describe a free particle, we require a relativistic equation having first order in time derivative like Schrodinger Equation but also treat space and time on equal footing for being Lorentz Invariant. **Paul Dirac** found the solution to this problem by giving Dirac equation which will be discussed in next section.

5 Dirac Equation

Dirac Equation is a relativistic wave equation which describes a single free particle having spin-$\frac{1}{2}$. It removes few of the shortcomings of Klein Gordon equation by defining a quantity called matrix square root in order to deal with the negative energy states problem.

5.1 The Dirac Equation

In order to remove the inconsistency in eq.(45) with the definition of probability density, we require an equation having linear relation between Energy and Momentum. From Einstein's Relation:

$$E^2 - \mathbf{p}^2 = m^2 \tag{46}$$

$$p^2 = p^\mu p_\mu = m^2 \tag{47}$$

Above equation is quadratic in E. Thus, Paul Dirac proposed to define a matrix square root $\not{p}$ where $\not{p}$ is the matrix square root of p^2. Defining

$$\boxed{\not{p} = \gamma^\mu p_\mu} \tag{48}$$

Applying this matrix square root on a wavefunction, we get,

$$\boxed{\not{p}\psi = m\psi} \tag{49}$$

$$\not{p}(\not{p}\psi) = \not{p}(m\psi) \tag{50}$$

$$\not{p}(\not{p}\psi) = m(\not{p}\psi) \tag{51}$$

$$\not{p}^2\psi = m^2\psi \tag{52}$$

$$p^2\psi = m^2\psi \tag{53}$$

Eq.(49) is linear relation between energy and momentum and thus it will be linear in space and time derivatives. It is also satisfying Einstein relation

∴ This equation is consistent with both the definition of probability density and special relativity and is called **Dirac Equation**.

5.2 Clifford Algebra

In eq.(48), γ^μ is four linearly independent matrices where, μ=0,1,2,3. It is independent of space and time.

∴ By definition

$$\not{p}\not{p} = p^2 \tag{54}$$

$$(\gamma^\mu p_\mu)(\gamma^\nu p_\nu) = p^2.\mathbb{1} \tag{55}$$

Since, γ^μ matrices are constant , therefore, they can be moved past momentum operators. Thus,

$$\gamma^\mu \gamma^\nu p_\mu p_\nu = p^2.\mathbb{1} \tag{56}$$

Replacing μ with ν and rewriting above equation,

$$\gamma^\nu \gamma^\mu p_\nu p_\mu = p^2.\mathbb{1} \tag{57}$$

Now adding eq.(56) and eq.(57) we get,

$$\gamma^\mu \gamma^\nu p_\mu p_\nu + \gamma^\nu \gamma^\mu p_\nu p_\mu = 2p^2.\mathbb{1} \tag{58}$$

Thus in order to satisfy above relation, we require

$$[\gamma^\mu, \gamma^\nu]_+ = 2\eta^{\mu\nu}.\mathbb{1} \tag{59}$$

This is called as Clifford Algebra. By this algebra, γ^μ matrices satisfies following properties:

- $$(\gamma^0)^2 = \mathbb{1} \tag{60}$$

- $$(\gamma^i)^2 = -\mathbb{1} \tag{61}$$

- $$\gamma^0\gamma^i + \gamma^i\gamma^0 = 0 \tag{62}$$

- $$\gamma^i\gamma^j + \gamma^j\gamma^i = 0 \quad \text{for} \quad i \neq j \tag{63}$$

- $$Tr(\gamma^0) = -Tr(\gamma^0) = 0 \tag{64}$$

- $$Tr(\gamma^i\gamma^0\gamma^i) = Tr(\gamma^i\gamma^i\gamma^0) \tag{65}$$

- The Dirac matrices are given as:

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -1 \end{pmatrix}, \tag{66}$$

$$\gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}, \tag{67}$$

5.3 Plane Wave solution of Dirac Equation

After finding the relativistic equation of our interest, we are concerned with finding the solution of that equation. Thus, Dirac Equation in eq.(49) can be rewritten as-

$$(\not{p} - m)\psi = 0 \tag{68}$$

$$(\gamma^{\mu} p_{\mu} - m)\psi = 0 \tag{69}$$

$$(i\gamma^{\mu} \partial_{\mu} - m)\psi = 0 \tag{70}$$

Here, eq.(69) is momentum representation and eq.(70) is coordinate representation.

Also, γ^{μ} is a (4x4) matrix and ψ is a (4x1) matrix. Assuming the solution of eq.(49) as:

$$\psi(x) = \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \\ \psi_4(x) \end{bmatrix} \tag{71}$$

It is seen that $\psi(x)$ is a multi-component wavefunction which suggests that there might be an **internal symmetry** in the system and also with the study of angular momentum, there might be a nontrivial spin angular momentum. But, since here, the system under consideration is simple and without having any internal symmetry, therefore, the solutions of Dirac Equations are expected to describe the **particles with spin**. The solution to Dirac Equation will be similar to plane wave equation as we are still dealing with single free particle:

$$\psi_\alpha(x) = e^{-ip\cdot x} u_\alpha(p), \quad \alpha = 1, 2, 3, 4 \tag{72}$$

Therefore, the matrix $u_\alpha(p)$ is given by a (4x1) column vector just like $\psi(x)$:

$$u(p) = \begin{pmatrix} u_1(p) \\ u_2(p) \\ u_3(p) \\ u_4(p) \end{pmatrix} \tag{73}$$

By putting eq.(73) in eq.(69) and expanding in terms of $\mu = 0, 1, 2, 3$, We get two positive and two negative energy solutions so, the energy eigenvalues are **doubly degenerate**.

The two independent solutions of wavefunction $\psi(x)$ are similar to the spin-up and spin-down states of the two component spinors given by:

$$u_+(p) = \begin{pmatrix} \tilde{u}(p) \\ \frac{\sigma\cdot\mathbf{p}}{E_+ + m}\tilde{u}(p) \end{pmatrix}, u_-(p) = \begin{pmatrix} \frac{\sigma\cdot\mathbf{p}}{E_- - m}\tilde{v}(p) \\ \tilde{v}(p) \end{pmatrix} \tag{74}$$

Note: σ is the Pauli spin matrices and

$$\tilde{u}(p) = \begin{pmatrix} u_1(p) \\ u_2(p) \end{pmatrix}, \quad \tilde{v}(p) = \begin{pmatrix} u_3(p) \\ u_4(p) \end{pmatrix} \tag{75}$$

$$p_0 = E_\pm = \pm(\sqrt{\mathbf{p}^2 + m^2}) \tag{76}$$

Note: In obtaining solution of Dirac Equation, we assumed that the motion of free particle in restricted to z-axis and therefore, $p_1 = p_2 = 0$.

Thus, it is proved that the solution of Dirac Equation describes the particle having spin (double degeneracy reflect the nontrivial spin structure of the wave function) (which was our assumption at the start of this section.)

5.4 Spin of Dirac Particles

The Pauli Spin matrices are given as:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{77}$$

The generalization of above matrices in 3D Euclidean space is given as:-

$$\tilde{\alpha}_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}, \quad i = 1, 2, 3 \tag{78}$$

We have free Dirac Hamiltonian given as:

$$H = \alpha \cdot \mathbf{p} + \beta . m \tag{79}$$

If the commutation relation between $\tilde{\alpha}$ and H is calculated, we get,

$$\begin{aligned} [\tilde{\alpha}_i, H] &= [\tilde{\alpha}_i, \alpha_j p_j + \beta m] \\ &= [\tilde{\alpha}_i, \alpha_j]\, p_j + [\tilde{\alpha}_i, \beta]\, m \\ &= 2i\epsilon_{ijk}\alpha_k p_j = -2i\epsilon_{ijk}\alpha_j p_k \end{aligned} \tag{80}$$

and since, the orbital angular momentum in Levi-Cevita form is defined as:

$$L_i = \epsilon_{ijk} x_j p_k \tag{81}$$

$\therefore$ commutation relation between L_i and H is calculated as:

$$\begin{aligned}[L_i, H] &= [\epsilon_{ijk} x_j p_k, \alpha_\ell p_\ell + \beta m] \\ &= [\epsilon_{ijk} x_j p_k, \alpha_\ell p_\ell] \\ &= \epsilon_{ijk} \alpha_\ell \left[x_j, p_\ell\right] p_k \\ &= \epsilon_{ijk} \alpha_\ell \left(i\delta_{j\ell}\right) p_k = i\epsilon_{ijk} \alpha_j p_k\end{aligned} \tag{82}$$

It is seen that none of the quantities in eq.(80) and eq.(82) is commuting with Hamiltonian. Now, If we calculate a quantity $L_i + \frac{1}{2}\tilde{\alpha}$, we get

$$[L_i + \frac{1}{2}\tilde{\alpha}_i, H] = 0 \tag{83}$$

As we know the total angular momentum commutes with Hamiltonian thus the quantity $\frac{1}{2}\tilde{\alpha}$ in eq.(83) is the spin angular momentum operator thereby making $J_i = L_i + S_i = 0$.

$$\therefore S_i = \frac{1}{2}\tilde{\alpha}_i \tag{84}$$

The theory describes the motion of free particle in z-axis, therefore

$$S_3 = \frac{1}{2}\tilde{\alpha}_3 = \frac{1}{2}\begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix} \tag{85}$$

The above matrix has doubly degenerate eigenvalues $\pm\frac{1}{2}$. Therefore, we reached on the conclusion that **Particles described by Dirac Equation corresponds to spin-$\frac{1}{2}$ particle.**

5.5 How Dirac resolved the inconsistency in probability density

This section describes how Dirac Equation overcomes the problem of Klein Gordon Equation of negative probability density.Writing it in Hamiltonian form as in eq.(86) and its complex conjugate in eq.(87),

$$i\frac{\partial\psi}{\partial t} = H\psi = (-i\alpha\cdot\nabla + \beta m)\psi \tag{86}$$

$$-i\frac{\partial\psi^\dagger}{\partial t} = \psi^\dagger(i\alpha\cdot\overleftarrow{\nabla} + \beta m) \tag{87}$$

Multiplying eq.(86) with $\psi^\dagger$ on the left and eq.(87) with ψ on the right and subtracting the two, we get

$$\frac{d}{\partial t}(\psi^\dagger\psi) = -\nabla.(\psi^\dagger\alpha\psi) \tag{88}$$

This is known as **'continuity equation"** for the probability current density. where

$$\rho = \psi^\dagger\psi = probability \quad density \tag{89}$$

$$\mathbf{J} = \psi^\dagger\alpha\psi = probability \quad current \quad density \tag{90}$$

so we can write

$$\frac{d\rho}{\partial t} = -\nabla.\mathbf{J} \tag{91}$$

This also suggest that we can write *current four vector* as

$$J^\mu = (\rho, \mathbf{J}) = (\psi^\dagger\psi, \psi^\dagger\alpha\psi) \tag{92}$$

so continuity equation in covariant form can be written as:

$$\partial_\mu J^\mu = 0 \tag{93}$$

This shows that the probability density (ρ) is the time component of J^μ and therefore, it must transform like the time coordinate under a Lorentz transformation.

On the other hand, the **total probability** is a constant and independent of any Lorentz transformation.

$$P = \int d^3x \psi^\dagger \psi \tag{94}$$

Thus, we conclude that although Dirac Equation (which is first order in time derivative) shows both positive and negative energy solutions, the probability density is **independent** of time derivative which was not the case with Klein Gordon equation.

5.6 Helicity

The Dirac Hamiltonian does not commute with either of L(orbital angular momentum) and S(spin angular momentum) but it commutes with the total angular momentum.

On the other hand, since momentum commutes with the Dirac Hamiltonian and so does $(S.p)$.

$$[S_i p_i, H] = [S_i, H] p_i = -\iota \epsilon_{ijk} \alpha_j p_k p_i = 0 \tag{95}$$

Therefore, this quantity is a constant of motion.

The normalized operator

$$\hat{h} = \frac{S.p}{|p|} \tag{96}$$

is the **projection of the spin along the direction of motion**.

This is known as the **"Helicity operator"**.

We can find its eigenvalues as

$$h^2 = \left(\frac{S.p}{|p|}\right)^2 = \frac{1}{4}\mathbb{1} \tag{97}$$

Therefore, the eigenvalues of the helicity operator can only be $\pm\frac{1}{2}$ for a Dirac particle.

5.7 Chirality

We have massless Dirac equation as

$$\not{p}u(p) = \not{p}v(p) = 0 \tag{98}$$

which has solution

$$u(p) = \sqrt{\frac{|\mathbf{p}|}{2}} \begin{pmatrix} \tilde{u}(p) \\ \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|}\tilde{u}(p) \end{pmatrix} \tag{99}$$

$$v(p) = \sqrt{\frac{|\mathbf{p}|}{2}} \begin{pmatrix} \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|}\tilde{v}(p) \\ \tilde{v}(p) \end{pmatrix} \tag{100}$$

Now, from dirac equation of massless particle, we can say that if u(p) is the solution then $\gamma_5 u(p)$ is also a solution.

Therefore, according to the eigenvalues of γ_5 the solutions of the massless Dirac equation can be classified also known as the **"Chirality"** or **"Handedness"**. This can also be seen from the fact that $H = \alpha.p$ (massless Dirac fermion) and γ_5 commutes.

Eigenvalues of γ_5 are ± 1.

Now we can **define**, spinors with the eigenvalue $+1$,

$$\gamma_5 u_R(p) = u_R(p), \quad \gamma_5 v_R(p) = v_R(p) \tag{101}$$

are known as **"right-handed"** (positive chirality) and spinors with the eigenvalue $+1$,

$$\gamma_5 u_L(p) = -u_L(p), \quad \gamma_5 v_L(p) = -v_L(p) \tag{102}$$

are known as **"Left-handed"** (Negative chirality).

Note: if the fermion is massive then the Dirac Hamiltonian will not commute with γ_5 and in this case we can not characterise spinors in terms of eigenvalues of γ_5.

If we have Given a general spinor, the right and left-handed components can be obtained through the *projection operators* as

$$u_R(p) = P_R u(p) = \frac{1}{2}(\mathbb{1} + \gamma_5) = \sqrt{\frac{|\mathbf{p}|}{2}} \begin{pmatrix} \frac{1}{2}(\mathbb{1} + \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{u}(p) \\ \frac{1}{2}(\mathbb{1} + \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{u}(p) \end{pmatrix} \tag{103}$$

$$u_L(p) = P_L u(p) = \frac{1}{2}(\mathbb{1} + \gamma_5) = \sqrt{\frac{|\mathbf{p}|}{2}} \begin{pmatrix} \frac{1}{2}(\mathbb{1} - \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{u}(p) \\ -\frac{1}{2}(\mathbb{1} - \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{u}(p) \end{pmatrix} \tag{104}$$

$$v_R(p) = P_R v(p) = \frac{1}{2}(\mathbb{1} + \gamma_5) = \sqrt{\frac{|\mathbf{p}|}{2}} \begin{pmatrix} \frac{1}{2}(\mathbb{1} + \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{v}(p) \\ \frac{1}{2}(\mathbb{1} + \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{v}(p) \end{pmatrix} \tag{105}$$

$$v_L(p) = P_L v(p) = \frac{1}{2}(\mathbb{1} + \gamma_5) = \sqrt{\frac{|\mathbf{p}|}{2}} \begin{pmatrix} -\frac{1}{2}(\mathbb{1} - \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{v}(p) \\ \frac{1}{2}(\mathbb{1} - \frac{\sigma\cdot\mathbf{p}}{|\mathbf{p}|})\tilde{v}(p) \end{pmatrix} \tag{106}$$

5.8 Limitations of Dirac Theory

As we have seen in the previous sections that if we describe a single particle by using quantum mechanics, we see so many difficulties arising due to it. The Relativistic particle has so much energy that it can create more particle-antiparticle pairs and thus theory consistent with above statement can't be a single particle theory.

Also, such theory is not adequate to describe various decay processes such as

$$n \to p + e^- + \overline{\nu_e}, \tag{107}$$

where distinct fermions are involved. Therefore, we need a multiparticle theory for dealing with these inconsistencies which is discussed in next section.

6 Classical Field Theory

If we want our theory to describe many degrees of freedom, then the very basic object to start building such a theory is a **field variable** which is a continuous function of space and time. From the study of the displacement field for the oscillations of a string, it is seen that such field variables lead to infinitely many modes of oscillation each of which can lead to a particle-like behavior upon quantization and, therefore, can describe many particles.

To start dealing with fields, we require a relativistic dynamical equation that must be invariant under Lorentz and Poincare´ transformation and then to quantize these fields.

6.1 Lagrangian Field Theory

Since, All the expressions in Lagrangian Formulation of field theory is explicitly Lorentz invariant, therefore, it is particularly suited for relativistic dynamics. So, We start with the very basic classical field theory-**the real scalar Klein Gordon theory**, and then quantize the dynamical variables as **operators** which obey canonical commutation relations.

Beginning with writing the **Action**, the fundamental quantity of classical mechanics:

$$S = \int_{t_i}^{t_f} L \; \mathrm{d}t \tag{108}$$

Here, L is the Lagrangian of classical scalar field which can be represented in terms of Lagrangian density $\mathcal{L}$ as

$$L = \int \mathrm{d}^3x \quad \mathcal{L} \tag{109}$$

So,

$$S = \int_{t_i}^{t_f} \mathrm{d}^4x \quad \mathcal{L} \tag{110}$$

Lagrangian density is the function of fields $\phi(x)$ and its derivatives $\partial_\mu \phi$.

According to Principle of Least Action, "when a system evolves from one point in space to another in time t_1 to t_2, it does so along the path that is extremum (either minimum or maximum). Classical trajectory of the particle is such that the Action (S) is stationary.
i.e.,

$$\delta S = 0 \tag{111}$$

If the field $\phi(x)$ is changed by an infinitesimal amount such as

$$\phi(x) \rightarrow \phi'(x) = \phi(x) + \delta\phi(x) \tag{112}$$

and subjected to boundary condition,

$$\delta\phi\,(\mathbf{x}, t_i) = \delta\phi\,(\mathbf{x}, t_f) = 0 \tag{113}$$

then we need to find under what condition the Action is Stationary?
So,

$$\delta S = \int_{t_i}^{t_f} \mathrm{d}^4x \quad \delta\mathcal{L} \tag{114}$$

$$\delta S = \int_{t_i}^{t_f} \mathrm{d}^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \delta\left(\partial_\mu \phi(x)\right) \right) \tag{115}$$

$$= \int_{t_i}^{t_f} \mathrm{d}^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) + \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \partial_\mu \delta\phi(x) \right) \tag{116}$$

$$= \int_{t_i}^{t_f} \mathrm{d}^4x \left[\frac{\partial \mathcal{L}}{\partial \phi(x)} \delta\phi(x) + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \delta\phi(x) \right) - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \delta\phi(x) \right] \tag{117}$$

$$= \int_{t_i}^{t_f} \mathrm{d}^4x \left(\frac{\partial \mathcal{L}}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \right) \delta\phi(x) + \int \mathrm{d}^3x \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)} \delta\phi(x) \Big|_{t_i}^{t_f} \tag{118}$$

Because of the boundary condition in eq.(113), the last term in eq.(118) vanishes, giving us the Euler lagrange Equation.

$$\left(\frac{\partial \mathcal{L}}{\partial \phi(x)} - \partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \right) = 0 \tag{119}$$

If we choose Lagrangian density to be

$$\mathcal{L} = \frac{1}{2}(\partial_\rho \phi)(\partial^\rho \phi) - \frac{m^2}{2}\phi^2 \tag{120}$$

then, the Euler-Lagrange equation will give Klein Gordon Equation for the free real scalar field as the dynamical equation.

$$\boxed{(\Box + m^2)\phi = 0} \tag{121}$$

We can also say that adding any constant term to L doesn't change equation of motion. If we make assumption that the fields are falling off rapidly at infinite separation, Action also won't change.

6.2 Hamiltonian Field Theory

Now, we need to develop Hamiltonian Description for the classical Klein Gordon field theory which is further quantized to build the Quantum field theory. Defining the canonical momenta for the field variable $\phi(x)$ as in eq.(122) and Hamiltonian density as in eq.(123),

$$\Pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)} \tag{122}$$

$$\mathcal{H} = \Pi(x)\dot{\phi}(x) - \mathcal{L} \tag{123}$$

where the Hamiltonian is

$$H = \int \mathrm{d}^3 x \mathcal{H} \tag{124}$$

Now, considering the Lagrangian of classical field as mentioned in eq.(101),

$$\mathcal{L} = \frac{1}{2}(\partial_\rho \phi)(\partial^\rho \phi) - \frac{m^2}{2}\phi^2 \tag{125}$$

The Hamiltonian obtained by putting this Lagrangian in eq.(122) and eq.(123) is

$$H = \int d^3 x \mathcal{H} = \int d^3 x \left[\frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2\right] \tag{126}$$

Calculating the dynamical equations from the above Hamiltonian, we get,

$$\dot{\phi}(x) = \Pi(x) \tag{127}$$

$$\dot{\Pi}(x) = \nabla \cdot \nabla\phi(x) - m^2\phi(x) = \nabla^2\phi(x) - m^2\phi(x) \tag{128}$$

These are the Hamiltonian equations which are first order equations. The second order equations obtained through it is

$$\ddot{\phi}(x) = \dot{\Pi}(x) = \nabla^2\phi(x) - m^2\phi(x) \tag{129}$$

$$\ddot{\phi}(x) - \nabla^2\phi(x) + m^2\phi(x) = 0 \tag{130}$$

$$(\partial^\mu\partial_\mu + m^2)\phi(x) = 0 \tag{131}$$

Therefore, we have obtained the classical Hamiltonian description of classical Klein Gordon field theory.

6.3 Quantization

Canonical Quantization is the tool to move from Hamiltonian formalism of classical theory to quantum theory. We take a generalised coordinate q_i and its conjugate momenta p^i and treat them operators. Therefore, applying it on fields, the quantization of this physical system will lead us to treat $\phi(x)$ and $\Pi(x)$ as Hermitian operators which must satisfy the following commutation relations,

$$\begin{aligned} &[\phi(x), \phi(y)]_{x^0=y^0} = 0 = [\Pi(x), \Pi(y)]_{x^0=y^0} \\ &[\phi(x), \Pi(y)]_{x^0=y^0} = i\delta^3(x-y) \end{aligned} \tag{132}$$

6.4 Field Decomposition

Considering the plane wave solution of classical field operator,

$$\phi(x) = \frac{1}{(2\pi)^{(3/2)}} \int d^3k e^{-\iota k.x} \tilde{\phi}(k) \tag{133}$$

If we put above solution in Klein Gordon equation we get two conditions:
Either $\tilde{\phi}(x) = 0$ or
$k^2 = m^2$ (which is known as the mass-shell condition).

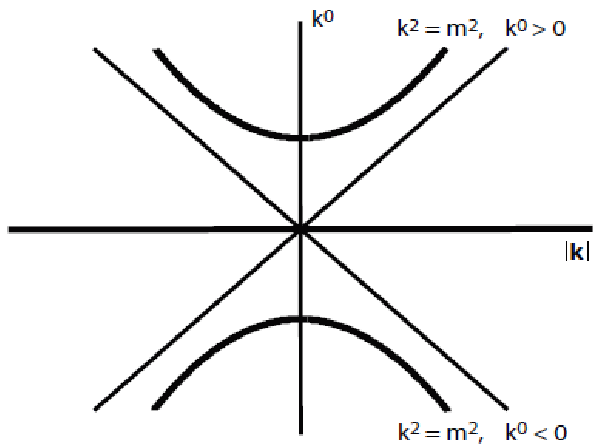


Figure 2: Mass shell on which $\tilde{\phi}(k)$ has support.

Therefore, combining the two conditions in one equation, we get,

$$\tilde{\phi}(k) = \delta(k^2 - m^2)a(k) \tag{134}$$

Putting this result back in eq.(133) and demanding $\phi^\dagger = \phi$, we arrive at the final expression of $\phi(x)$ in terms of creation and annihilation operators:

$$\phi(x) = \int \frac{d^3k}{\sqrt{(2\pi)^3 2k^0}}(e^{-\iota k.x}a(\mathbf{k}) + e^{\iota k.x}a^\dagger(\mathbf{k})) \tag{135}$$

where,

$$a(\mathbf{k}) = \frac{a(k)}{\sqrt{2k^0}}, \quad a^\dagger(\mathbf{k}) = \frac{a^\dagger(k)}{\sqrt{2k^0}} \tag{136}$$

Thus, the expression for the field operator shows its decomposition into positive and negative energy states.

$$\phi(x) = \phi^+(x) + \phi^-(x) \tag{137}$$

6.4.1 Commutation Relations of Creation and Annihilation Operators

Since, the canonical momenta is defined as,

$$\Pi(x) = \dot{\phi} = \int d^3k(-\iota)\sqrt{\frac{k^0}{2(2\pi)^3}}(e^{-\iota k.x}a(\mathbf{k}) - e^{\iota k.x}a^\dagger(\mathbf{k})) \tag{138}$$

Imposing the quantization relations between $\phi(x)$ and $\Pi(x)$ we get,

$$[\phi(x), \phi(y)]_{x^0=y^0=0} = 0 \tag{139}$$

$$[\Pi(x), \Pi(y)]_{x^0=y^0=0} = 0 \tag{140}$$

$$[\phi(x), \Pi(y)]_{x^0=y^0=0} = \iota\delta^3(x-y) \tag{141}$$

With the use of above commutation relations we obtain the commutation relation between $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$

$$[a(\mathbf{k}), a(\mathbf{k'})] = [a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k'})] = 0 \tag{142}$$

$$[a(\mathbf{k}), a^\dagger(\mathbf{k'})] = \delta^3(k-k') \tag{143}$$

6.5 Klein Gordon Theory as Harmonic Oscillators

Looking at the mass-shell support of $\tilde{\phi}(x)$, we can say that the most general solution of Klein Gordon equation is a linear superposition of simple harmonic oscillators, each vibrating at a different frequency and amplitude. In order to quantize this field $\phi(x)$ we simply quantize this infinite number of harmonic oscillators.[8] Recalling the Hamiltonian,

$$H = \int d^3x \left[\frac{1}{2}\Pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2\right] \tag{144}$$

Now using $\phi(x)$ and $\Pi(x)$ in Hamiltonian we get,

$$H = \int d^3k \frac{E_k}{2}(a(\mathbf{K})a^\dagger(\mathbf{K}) + a^\dagger(\mathbf{K})a(\mathbf{K})) \tag{145}$$

We can calculate some commutation relations which is found to be analogous to linear harmonic oscillator.

$$[a(\mathbf{k}), H] = E_k a(\mathbf{k}) \tag{146}$$

$$[a^\dagger(\mathbf{k}), H] = -E_k a^\dagger(\mathbf{k}) \tag{147}$$

Defining number operator

$$N(\mathbf{k}) = a^\dagger(\mathbf{k})a^(\mathbf{k}) \tag{148}$$

and from the result:

$$[a(\mathbf{k}), a^\dagger(\mathbf{k})] = \delta^3(0) \tag{149}$$

we see a dirac delta function coming in Hamiltonian which give rise to infinity spike. Thus, in order to deal with this type of ambiguity, Normal ordering is applied which puts the operators in the order such as the creation operator is always to the left of annihilation operator.

$$(a(\mathbf{k})a^\dagger(\mathbf{k}))^{N.O.} = a^\dagger(\mathbf{k})a(\mathbf{k}) \tag{150}$$

The Hamltonian then becomes

$$H = \int d^3k \quad E_k \quad a^\dagger(\mathbf{K})a(\mathbf{K}) \tag{151}$$

7 Green Function

It propagates the particle from one spacetime point to other. It is a method to find the solution of differential equation.
consider a differential equation

$$\hat{L}x(t) = f(t) \tag{152}$$

where $\hat{L}$ is a differential operator.
We **define** Green function **G(t,u)** of $\hat{L}$ as

$$\hat{L}G(t,u) = \delta(t-u) \tag{153}$$

where u as a dummy variable. The solution x(t) is given by

$$x(t) = \int G(t,u)f(u)du \tag{154}$$

We can verify that this is indeed the solution by operating $\hat{L}$ on x(t),

$$\hat{L}x(t) = \int \hat{L}G(t,u)f(u)du \tag{155}$$

Now from equation (156)

$$\hat{L}x(t) = \int \delta(t-u)f(u)du \tag{156}$$

$$\hat{L}x(t) = f(t) \tag{157}$$

Therefore, we can solve non-homogeneous differential equations by finding Green's Function **G(t,u)** and then integrating over f(u) to get the solution, i.e., x(t).

8 Causality

Taking into account the requirement for fields which was discussed at the start of this paper,i.e.,Causality. For any theory to be causal, it requires that all spacelike separated operators must commute. Mathematically

$$[\hat{O}(x_1), \hat{O}(x_2)] = 0 \quad (x-y)^2 < 0 \tag{158}$$

It ensures that a measurement at x should not affect the measurement at y when the separation of x and y are spacelike.

In order to check if the operators we are working with satisfies this crucial property or not, Let us define

$$\Delta(x-y) = [\hat{\phi}(x), \hat{\phi}(y)] \quad \text{for all} \quad (x-y)^2 < 0 \tag{159}$$

By substituting in above equation, we find that $\Delta(x-y)$ is a complex number function.

$$\Delta(x-y) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_p} (e^{-\iota p.(x-y)} + e^{\iota p.(x-y)}) \tag{160}$$

By looking at the above expression ,it can be inferred that

- It is Lorentz invariant because of $\int \frac{d^3p}{2E_p}$ being L.I.
- It doesn't vanish for timelike separation, $\Delta(x-y) = e^{-}imt + e^{+}imt$
- It vanishes for space-like separations, $\Delta(x-y) = 0$

Therefore our theory is causal having the commutation relations vanishing outside the lightcone.

9 Propagator

Propagators are the Green's Function of the equation of motions for a particle.[8] If we prepare a particle at spacetime point y then what is the amplitude to find it at point x?

Mathematically this can be expressed as

$$\langle 0| \phi(x)\phi(y) |0\rangle = \int \frac{d^3p}{(2\pi)^3}\frac{d^3p'}{(2\pi)^3}\frac{1}{(\sqrt{2E_p})(\sqrt{2E'_p})} \langle 0| a_p a_p^{\dagger\prime} |0\rangle \, e^{-\iota p.x+\iota p'.y} \tag{161}$$

$$= \int \frac{d^3pd^3p'}{(2\pi)^6}\frac{1}{(\sqrt{2E_p})(\sqrt{2E'_p})} \langle p|p'\rangle \, e^{-\iota p.x+\iota p'.y} \tag{162}$$

$$= \int \frac{d^3pd^3p'}{(2\pi)^6}\frac{1}{\sqrt{4E_pE'_p}}(2\pi)^3\delta^3(p-p')e^{-\iota p.x+\iota p'.y} \tag{163}$$

$$= \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\vec{p}}}e^{-\iota p.(x-y)} \equiv D(x-y) \tag{164}$$

$D(x-y)$ is known as **Propagator**.

<u>CASE:1</u> For timelike separation, $x^0 - y^0 = t$ and $\mathbf{x} - \mathbf{y} = 0$

$$D(x-y) = \frac{4\pi}{(2\pi)^3}\int_0^\infty dp \frac{p^2}{2\sqrt{p^2+m^2}}e^{-i\sqrt{p^2+m^2}t} \tag{165}$$

$$= \frac{1}{4\pi^2}\int_m^\infty dE\sqrt{E^2-m^2}e^{-iEt} \tag{166}$$

$$\sim e^{-imt} \quad as \quad t \to \infty \tag{167}$$

<u>CASE:2</u> For spacelike separation, $x^0 - y^0 = 0$ and $\mathbf{x} - \mathbf{y} = \mathrm{r}$

$$D(x-y) = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}e^{-i\mathbf{p}\cdot 0+\iota\mathbf{p}\cdot\mathbf{r}} \tag{168}$$

$$D(x-y) \sim e^{-mr} \tag{169}$$

To calculate D(x-y) for spacelike separation,

The integrand, which is a complex function of p, has branch cut imaginary axis starting at $\pm im$. To evaluate it, the contour is pushed up to wrap around the upper branch cut.

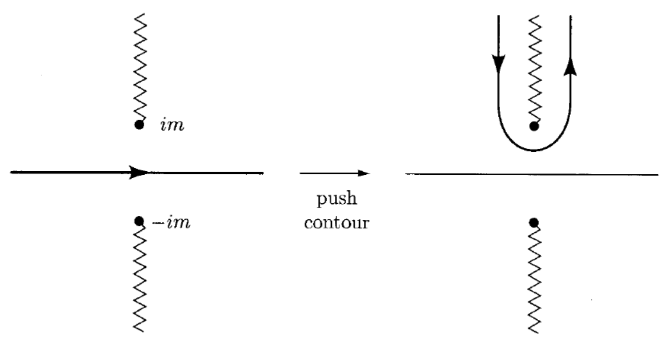


Figure 3: Contour for evaluating D(x-y) for spacelike.

It is coming out to be non-vanishing for spacelike separation.But we've previously discussed that spacelike measurements commute and the theory is causal. ∴ We can write

$$[\hat{\phi}(x), \hat{\phi}(y)] = D(x-y) - D(y-x) = 0 \quad \text{for} \quad (x-y)^2 < 0 \tag{170}$$

For a complex scalar field, Requiring that $(x-y) \rightarrow -(x-y)$ such that the amplitude of a particle going from y to x cancels out the amplitude of antiparticle travelling from x to y. Thus, Causality is preserved.

9.1 Feynman Propagator

In order to study the interacting fields, Feynman introduced this quantity which has the contribution of both particle and antiparticle parts and is very important for calculating the amplitudes of various scattering experiments. He applied

Wick's ordering and defined the quantity as

$$\Delta_F(x-y) = \langle 0| T\phi(x)\phi(y) |0\rangle = \begin{cases} D(x-y) & \text{if } x^0 > y^0 \\ D(y-x) & \text{if } y^0 > x^0 \end{cases} \tag{171}$$

where T is time ordering.

by placing operators evaluated at later times to the left

$$T\phi(x)\phi(y) = \begin{cases} \phi(x)\phi(y) & x^0 > y^0 \\ \phi(y)\phi(x) & y^0 > x^0 \end{cases} \tag{172}$$

Claim: The mathematical expression of feynman propagator is given by

$$\Delta_F(x-y) = \int \frac{d^4p}{(2\pi)^4} \frac{\iota}{p^2 - m^2} e^{-\iota p.(x-y)} \tag{173}$$

This expression contains poles at $p^0 = \pm E_{\vec{p}} = \pm\sqrt{\vec{p}^2 + m^2}$

So we need a prescription for avoiding these singularities in the p^0 integral. So we must choose the contour as

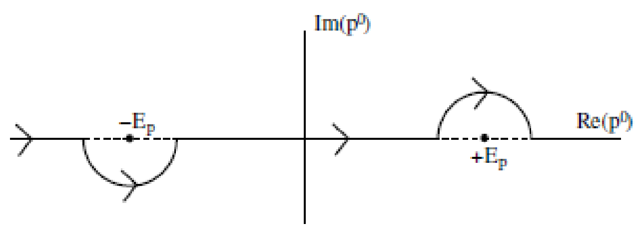


Figure 4: Contour for the Feynman Propagator.

Proof: The residue of the pole at $p^0 = \pm E_{\vec{p}}$ is $\pm\frac{1}{2E_{\vec{p}}}$

case 1: when $x^0 > y^0$

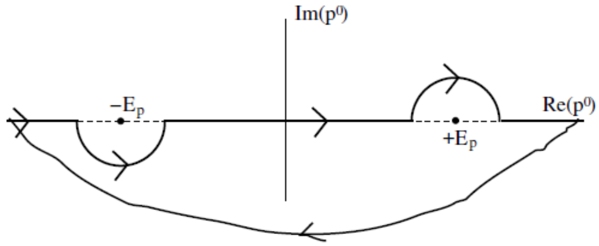


Figure 5: Contour for $case : x^0 > y^0$.

$$\Delta_F(x-y) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_{\vec{p}}} e^{-\iota p.(x-y)} = D(x-y) \tag{174}$$

case 2: when $y^0 > x^0$

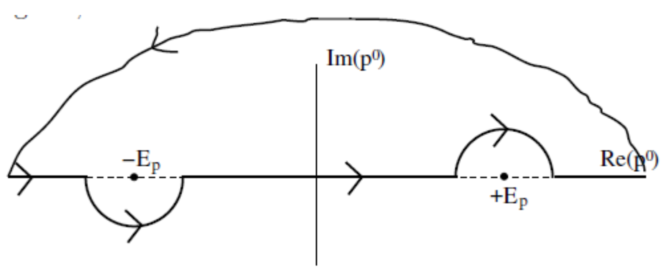


Figure 6: Contour for $case : y^0 > x^0$.

$$\Delta_F(x-y) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_{\vec{p}}} e^{-\iota p.(y-x)} = D(y-x) \tag{175}$$

9.2 Feynman Propagator as Green's function for the Klein-Gordon Equation

$$(\partial_t^2 - \nabla^2 + m^2)\Delta_F(x-y) = \int \frac{d^4p}{(2\pi)^4} \frac{\iota}{p^2 - m^2}(-p^2 + m^2)e^{-\iota p.(x-y)} \tag{176}$$

$$= -\iota\delta^4(x-y) \tag{177}$$

Therefore, Feynman Propagator is Green's function for the Klein-Gordon Equation.

10 S-matrix

The S-matrix is like the time-evolution operator for interaction picture. It is the basic building block of Quantum Field theory. Scattering is one of the interaction process. At the start of the scattering experiment, particles are far apart from each other, they interact for a short period of time and then again goes apart. Working in the Heisenberg picture, it is very complicated to write down convincing expressions for the time-dependent operators for such interactions.

[5]$SoWheelersuggestedthat, wesplitintotwoparts = {}_0 + \hat{H}'$, where $\hat{H}_0$ describes a **simple world** of non-interacting particles described by some set of state vectors. Since, we're working in the Heisenberg picture, these state vectors don't change at all.

Now, writing simple world states for two particles as momentum states (before the interaction) $|p_2p_1\rangle_{sw}$. Now, there is a similar state in "real world" at $t \to -\infty$. we will call this $|p_2p_1\rangle_{rw}^{in}$ or **in state** .

similarly we have $|q_2q_1\rangle_{sw}$ (after the ineraction) and there is a similar state in "real world" at $t \to \infty$. we will call this $|p_2p_1\rangle_{rw}^{out}$ or **out state**.

For the real-world scattering process the amplitude $\mathcal{A}$ for starting with $|p_2p_1\rangle_{rw}^{in}$ and ending up with $|q_2q_1\rangle_{rw}^{out}$ is given by

$$\mathcal{A} = {}_{rw}^{out}\langle q_1q_2|p_2p_1\rangle_{rw}^{in} \tag{178}$$

Now, we need to change this "real world" states into "simple world" states as those are the ones which we can evaluate without any complications.

Wheeler's used the S-matrix to calculate this amplitude in simple world without involving interactions.

$$A = {}^{in}_{rw} \langle q_2 q_1 | p_2 p_1 \rangle^{out}_{rw} = {}_{sw} \langle q_2 q_1 | \hat{S} | p_2 p_1 \rangle_{sw} \tag{179}$$

In order to calculate such amplitudes, we need two things:

- A way of getting a $\hat{H}_0$ to describe simple-world states which resemble the 'in' and 'out' states.
- A way of calculating an expression for the $\hat{S}$-operator.

Finding the suitable $\hat{H}_0$ is achieved by new formulation called **Interaction Representation**.

10.1 Interaction Representation

In Schrodinger picture, we treat operators as time-independent and states as time-dependent. But here we are working in Heisenberg picture, So, we treat states as time-independent whereas the operators as time-dependent. Cosnidering the free part of Hamiltonian (H_0)

$$\hat{\mathcal{O}}_I(t) = e^{\iota \hat{H}_0 t} \hat{\mathcal{O}} e^{-\iota \hat{H}_0 t} \tag{180}$$

The key points of this representation are:

- Both, operators and states can evolve in time.
- operators evolve via free part of the Hamiltonian

$$\hat{\phi}_I(t) = e^{\iota \hat{H}_0 t} \hat{\phi} e^{-\iota \hat{H}_0 t} \tag{181}$$

- states evolve via interacting part of the Hamiltonian

$$\iota \frac{\partial}{\partial t} |\psi(t)\rangle_I = \hat{H}_I(t) |\psi(t)\rangle_I \tag{182}$$

$$\hat{H}_I = e^{\iota \hat{H}_0 t} \hat{H}' e^{-\iota \hat{H}_0 t} \tag{183}$$

Note: All different representations coincide at t=0.

10.2 Interaction Picture applied to Scattering

While working in interaction picture, We consider interaction part of Hamiltonian (H') to be zero at the start and the end of the experiment. This leaves us only with the free part of Hamiltonian (H_0) for $t \to \pm\infty$. Therefore we can write

$$|\phi\rangle_{sw} = |\phi_I(\pm\infty)\rangle \tag{184}$$

These states are the eigenstates of H_0 and we can canonically quantize them and obtain the eigenvalues. Since all quantum mechanical pictures are defined so that they coincide at t = 0, we can write

$$_{sw}\langle\phi|\, \hat{S}\, |\psi\rangle_{sw} = {}^{out}_{rw}\langle\phi|\psi\rangle^{in}_{rw} = \langle\phi_I(0)|\psi_I(0)\rangle \tag{185}$$

Now, if we have the time-evolution operator in the interaction picture $\hat{U}_I(t_2, t_1)$, we could say that

$$_{sw}\langle\phi|\, \hat{S}\, |\psi\rangle_{sw} = \langle\phi_I(\infty)|\, \hat{U}_I(\infty, 0)\hat{U}_I(0, -\infty)\, |\psi_I(-\infty)\rangle \tag{186}$$

Now from equation (184)

$$_{sw}\langle\phi|\, \hat{S}\, |\psi\rangle_{sw} = {}_{sw}\langle\phi|\, \hat{U}_I(\infty, -\infty)\, |\psi\rangle_{sw} \tag{187}$$

Therefore, $\hat{S}$ is the **time-evolution operator for the interaction-picture** as $t \to \infty$

10.3 Perturbation Expansion of the S-matrix

Like Schrodinger picture, we have an equation of motion of time-evolution operator in the interaction picture.

$$\iota\frac{\partial}{\partial t_2}\hat{U}_I(t_2,t_1)=\hat{H}_I(t_2)\hat{U}_I(t_2,t_1) \tag{188}$$

We also have

$$[\hat{H}_I(t_2),\hat{H}_I(t_1)]\neq 0 \tag{189}$$

Therefore we need to use **time-ordered product** as everything within a time-ordered product commutes.

The expression for $\hat{U}(t_2,t_1)$ is given by **Dyson's expansion**. Therefore, the solution of eq.(188) is

$$\hat{U}(t_2,t_1)=T[e^{-\iota\int_{t_1}^{t_2}dt\hat{H}_I(t)}] \tag{190}$$

This is called **Dyson Expansion** As we already know that $\hat{S}$-operator is also a time evolution operator therefore,

$$\hat{S}=T[e^{-\iota\int_{t_1}^{t_2}d^4x\hat{\mathcal{H}}_I(x)}] \tag{191}$$

The perturbation expansion of this expression can be obtained as:

$$\hat{S}=T\left[1-\mathrm{i}\int\mathrm{d}^4z\hat{\mathcal{H}}_{\mathrm{I}}(z)+\frac{(-\mathrm{i})^2}{2!}\int\mathrm{d}^4y\ \mathrm{d}^4w\hat{\mathcal{H}}_{\mathrm{I}}(y)\hat{\mathcal{H}}_{\mathrm{I}}(w)+\dots\right] \tag{192}$$

provided that $\mathcal{H}_I$ is small compared to total hamiltonian

10.4 Wick's Theorem

This theorem is used to solve long strings of operators that appear in Dyson expansions. In place of calculating vacuum expectation value(VEV) of the time ordered string of operators $\langle 0| T[\hat{A}\hat{B}....\hat{Z}] |0\rangle$, it is easier to calculate the VEV of normal ordered strings of operators $\langle 0| T[\hat{A}\hat{B}....\hat{Z}] |0\rangle$ as it places a to the right of $a^{\dagger}$, thus giving VEV as zero. The field has two parts such as

$$\hat{\phi} = \hat{\phi}^{-} + \hat{\phi}^{+} \tag{193}$$

Calculating the relation between the time ordered and normal ordered string of operators, we have

$$\hat{A}\hat{B} - N[\hat{A}\hat{B}] = [\hat{A}^{-}, \hat{B}^{+}] \tag{194}$$

$$T[\hat{A}(x)\hat{B}(y)] - N[\hat{A}(x)\hat{B}(y)] = \begin{cases} [\hat{A}^{-}(x), \hat{B}^{+}(y)] & \text{if } x^0 > y^0 \\ [\hat{B}^{-}(y), \hat{A}^{+}(x)] & \text{if } y^0 > x^0 \end{cases} \tag{195}$$

Since the VEV of a normal ordered product is zero

$$\langle 0| T[\hat{A}(x)\hat{B}(y)] |0\rangle = \begin{cases} [\langle 0| \hat{A}^{-}(x), \hat{B}^{+}(y) |0\rangle] & \text{if } x^0 > y^0 \\ [\langle 0| \hat{B}^{-}(y), \hat{A}^{+}(x) |0\rangle] & \text{if } y^0 > x^0 \end{cases} \tag{196}$$

If $\hat{A} = \hat{B} = \hat{\phi}$, then the quantity on the left is Feynman propagator. Therefore we define the commutator as **Contraction** like:

$$\overbracket{AB} = T[\hat{A}\hat{B}] - N[\hat{A}\hat{B}] \tag{197}$$

since contraction is a commutation relation, Therefore it is just a complex number.

By taking VEV both sides we find that

$$\overbrace{AB} = \langle 0| T[\hat{A}\hat{B}] |0\rangle \tag{198}$$

Therefore

$$T[\hat{A}\hat{B}] = N[\hat{A}\hat{B} + \overbrace{AB}] \tag{199}$$

More Generally

$$T[\hat{A}\hat{B}...\hat{Z}] = N[\hat{A}\hat{B}...\hat{Z} + (All \quad possible \quad contraction \quad of \quad \hat{A}\hat{B}...\hat{Z})] \tag{200}$$

This is known as Wick's theorem and is very useful for calculating commutation relation between various long strings of operators.

11 Expanding S-Matrix as Feynman Propagators

The terms in perturbation expansion of S-Matrix can be represented by Feynaman Diagrams.

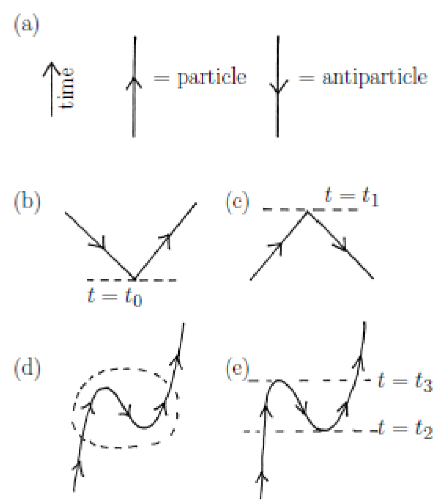


Figure 7: The Feynman diagram. (a) A particle is represented by a line with an arrow going in the direction of time (conventionally up the page). An antiparticle is represented by a line with an arrow going the opposite way. (b) A particle and antiparticle created at time t = t0. (c) A particle and antiparticle are annihilated at time t = t1. (d) Trajectory of a single particle can be interpreted as follows: (e) A particle– antiparticle pair are created at t2, the antiparticle of which annihilates with a third particle at t = t3.

11.1 Example of ϕ^4 Theory

In this section we try to calculate an S-matrix element for ϕ^4 theory.

Consider the Lagrangian

$$L = \frac{1}{2}(\partial_\mu \phi)^2 - \frac{1}{2}m^2\phi^2 - \frac{\lambda}{4!}\phi^4 \tag{201}$$

Now we will try to find S-matrix in the following steps

- **Step 1**

  we will choose 'in' and 'out' state to be a single particle momentum state p and q respectively.

  we calculate the amplitude as

$$A = {}^{out}\langle q|p\rangle^{in} = \langle q|\hat{S}|p\rangle \tag{202}$$

$$= (2\pi)^3(2E_q)^{1/2}(2E_p)^{1/2}\langle 0|\hat{a}_p\hat{S}\hat{a}_p^\dagger|0\rangle \tag{203}$$

- **Step 2**

  We will do the Dyson's expansion

$$\hat{S} = T\Big[1 - \frac{\iota\lambda}{4!}\int d^4z\hat{\phi}^4(z) + \frac{(-\iota\lambda)^2}{2!}\frac{\lambda}{4!}^2\int d^4yd^4w\hat{\phi}^4(y)\hat{\phi}^4(w) + ...\Big] \tag{204}$$

- **Step 3**

  putting $\hat{S}$ in amplitude A

$$A = (2\pi)^3(2E_q)^{1/2}(2E_p)^{1/2}T\Big[\langle 0|a_qa_p^\dagger|0\rangle - \frac{\iota\lambda}{4!}\int d^4z\langle 0|a_q\hat{\phi}^4(z)a_p^\dagger|0\rangle + \frac{(-\iota\lambda)^2}{2!}\frac{\lambda}{4!}^2\int d^4yd^4w\langle 0|a_q\hat{\phi}^4(y)\hat{\phi}^4(w)a_p^\dagger|0\rangle + ...\Big]$$

  we can also write this as

$$A = A^{(0)} + A^{(1)} + A^{(2)}.... \tag{205}$$

- **Step 4**

  Using wick's theorem, we calculate various expectation values.

  Combining all the permutations of $\hat{a} - \phi$ contractions and the $\phi - \phi$ contractions separately, the amplitude $A^{(1)}$ can be written as

$$A^{(1)} = -\frac{\iota\lambda}{4!}\int d^4z \Big[3\langle 0|\,\hat{a}_q\hat{a}_p^\dagger\,|0\rangle\,\langle 0|\,\hat{\phi}(z)\hat{\phi}(z)\,|0\rangle\,\langle 0|\,\hat{\phi}(z)\hat{\phi}(z)\,|0\rangle$$
$$+12\,\langle 0|\,\hat{a}_q\hat{\phi}(z)\,|0\rangle\,\langle 0|\,T\hat{\phi}(z)\hat{\phi}(z)\,|0\rangle\,\langle 0|\,\hat{\phi}(z)\hat{a}_p^\dagger\,|0\rangle\Big]$$

- **Step 5** In this section we will draw the feynman diagram of the expression which appears in the amplitude.

  The rules for drwaing the diagrams are as follows:

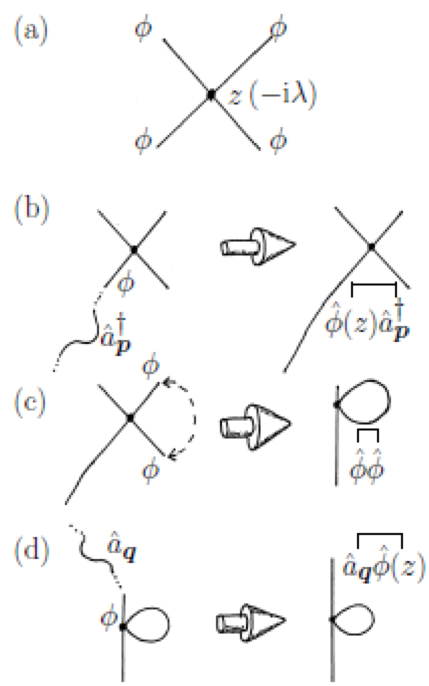


Figure 8: Feynman Diagram.

  - Drawing the interaction vertices and labelling them with their space-time coordinates as in fig (a)
  - Contractions between the initial state and a field, i.e. $\overbracket{\phi(x)a_p^\dagger}$ are

drawn as incoming lines connecting to one of the legs of the vertex Fig(b). This corresponds to a real, on-mass-shell particle coming inside.

- Propagators resulting from the field–field contractions $\phi(x)\phi(x)$ are drawn as lines linking the points [Fig(c)].These are thought of as **virtual particles** which are internal to the story the diagram is telling.
- Contractions between the final state and a field $a_q\phi(x)$ are drawn as an outgoing lines as in [Fig(d)]. These correspond to **on-mass shell** particles going out.

The connected and disconnected diagrams are shown below:

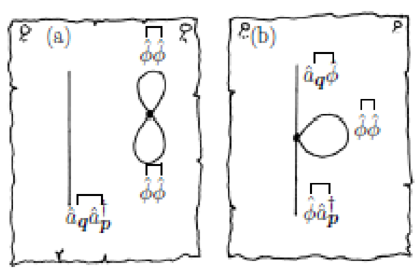


Figure 9: Connected and Disconnected Feynman Diagrams

- Left figure is Disconnected Diagram. They don't influence each other and only contribute to the phase of transition amplitudes
- Right figure is for connected diagram. It doesnt affect the transition probabilities.

IV Semester: Introduction

The out-of-time-order correlator (OTOC) is considered as a determination tool of quantum chaos. By making small changes in the initial conditions,the exponential growth of the OTOC in its time evolution is regarded as the indicator of the chaos. Traditional indicator is energy level spacings, and we are interested is finding out if the OTOC can be a better indicator of quantum chaos or not. OTOCs are gaining attention these days because it can be an indicator of possible gravity dual, through the AdS/CFT correspondence.[6, 7]

We are taking a system of two harmonic oscillators coupled non-linearly with each other, in eq.(206) and we will see the chaotic behavior in this system on increasing the energy eigenvalues.[1] Poincare sections shown in fig.(10) shows the chaotic behavior in classical CHO. We , further, discuss the analytical method for computing OTOC in quantum mechanical system and will apply that technique in reproducing the graph showing variation of microcanonical OTOC as in fig.(14).

$$H = \left(p_x^2 + \frac{1}{4}\omega^2 x^2\right) + \left(p_y^2 + \frac{1}{4}\omega^2 y^2\right) + g_0 x^2 y^2 \tag{206}$$

Applying the numerical technique of section (12.2), the OTOC for a 1D Harmonic Oscillator comes out to be **Oscillatory**. More complicated examples that exhibit classical chaos such as the two-dimensional stadium billiard give OTOCs that are growing non-exponentially at early times followed by a saturation at late times.[4] Early-time exponential growth of OTOCs has been found in a system of non-linearly coupled oscillators, which is expected to exhibit quantum chaos. We also plot the energy eigenvalue variation of anharmonic oscillator with n and plot the microcanonical OTOC for an anharmonic oscillator.[9]

12 Classical Chaos in the Coupled Harmonic Oscillators

In equation 206, we have potential as

$$U(x,y) = \frac{\omega^2}{4}(x^2 + y^2) + g_0 x^2 y^2 \tag{207}$$

with $\omega = 1, g_0 = 0.1$

At low energy values, the system eq.(207) is in regular phase and At high energy values, in chaotic phase and this behavior is shown regardless of whether the system is classical or quantum. Looking at the potential U(x,y), the system acts as a 2D harmonic oscillator at low energy. On the other hand, at the high energy, the energy contribution of the non-linear term becomes significant and this system turns into chaotic.

The chaotic behavior for a classical system is determined by Poincare sections and Lyapunov exponents.

Quantum mechanically, chaos is analysed by the nearest-neighbor spacings of the energy eigenvalues of the system.

For **Quantum systems**, OTOC is another quantity to discriminate a quantum chaos. The **Quantum Lyapunov Exponent** is the quantitative indicator, which measures the exponential growth of the OTOC.

12.1 Poincare Surface of Sections for Classical Coupled Harmonic Oscillator

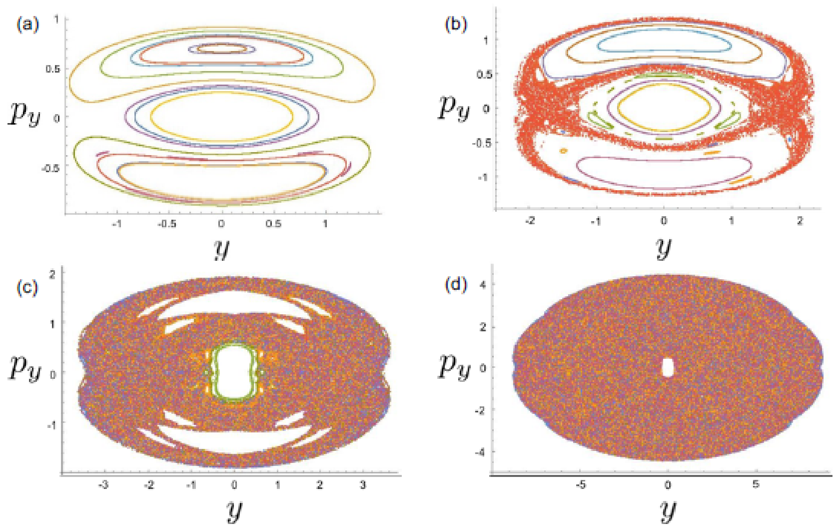
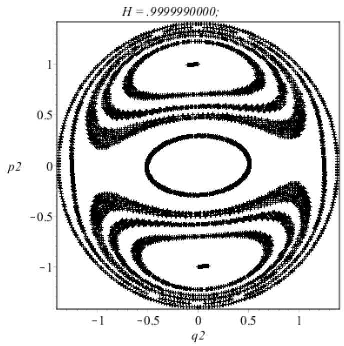
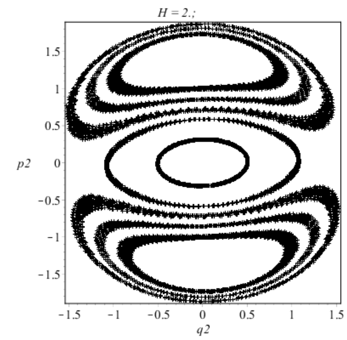


Figure 10: Poincare Surface of Sections for Coupled Harmonic Oscillator

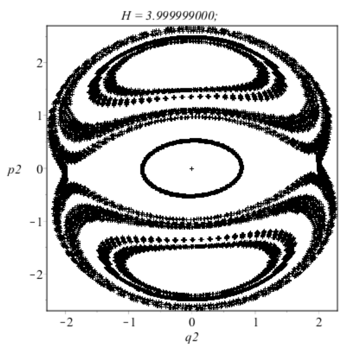
We reproduced the graph as in fig.11 using Maple Software. It is seen that on increasing the energy, the orbits are getting destroyed and becoming more and more chaotic for higher energy values.



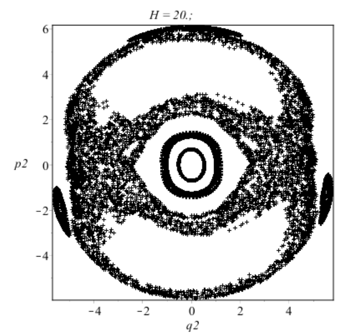
(a) E=1



(b) E=2



(c) E=4



(d) E=20

Figure 11: Poincare Surface of Sections for Coupled Harmonic Oscillator plotted on Maple Software

In the figure, subfigure (a), (b), (c) and (d) correspond to E = 1; 2; 4 and 20 respectively. At a low energy, we can clearly see the orbits in the Poincaré section, which indicates that the system is in a regular phase. On the other hand the orbits are destroyed and the Poincaré section is filled with scattered plots for high energy which reflects that the system is in a chaos phase.

12.2 Numerical Computation technique for calculating OTOC

Time independent Hamiltonian :

$$H \equiv H(x_1, x_2, ...x_n, p_1, p_2....p_n) \tag{208}$$

OTOC is defined as

$$C_T(t) = - < [x(t), p(0)]^2 > \tag{209}$$

We know,

$$< \mathcal{O} > \equiv \frac{tr[e^{-\beta H}\mathcal{O}]}{tr[e^{-\beta H}]} \tag{210}$$

Also,

$$tr(\hat{A}) = \sum \langle n| \hat{A} |n\rangle \tag{211}$$

$$A_{mn} = \langle m| \hat{A} |n\rangle \tag{212}$$

Using the definition of expectation value given by (210) in (209), we get

$$C_T(t) = -\frac{tr[e^{-\beta H}[x(t), p(0)]^2]}{tr[e^{-\beta H}]} \tag{213}$$

$$C_T(t) = -\frac{tr[e^{-\beta H}[x(t), p(0)]^2]}{Z} \tag{214}$$

since $\mathbf{Z} = \mathbf{tr}[\mathbf{e}^{-\beta\mathbf{H}}]$ is the partition function. Using (211) in (214) we get,

$$C_T(t) = -\frac{1}{Z}\sum_n \langle n| e^{-\beta E_n}[x(t), p(0)]^2 |n\rangle \tag{215}$$

$$= -\frac{1}{Z}\sum_n e^{-\beta E_n} \langle n| [x(t), p(0)]^2 |n\rangle \tag{216}$$

$$= -\frac{1}{Z}\sum_n e^{-\beta E_n} c_n(t) \tag{217}$$

Here, $c_n(t) = \langle n| [x(t), p(0)]^2 |n\rangle$ is microcanonical OTOC for fixed energy eigenstate and $C_T(t)$ is the thermal OTOC.

$$c_n(t) = \sum_m (-\iota^2) \langle n| [x(t), p(0)] |m\rangle \langle m| [x(t), p(0)] |n\rangle \tag{218}$$

The completeness condition $|n\rangle \langle n| = 1$ brings the microcanonical OTOC $c_n(t)$ in to the following form:

$$c_n(t) = \sum_m b_{nm}(t) b^*_{nm}(t) \tag{219}$$

where $b_{nm} = -\iota \langle n| [x(t, p(0)] |m\rangle$ Substituting $x(t) = e^{\iota Ht} x e^{-\iota Ht}$ to the expression of $b_{nm}(t)$ and using the completeness condition again, we obtain

$$b_{nm}(t) = -\iota \langle n| [e^{\iota Ht} x e^{-\iota Ht}, p(0)] |m\rangle \tag{220}$$

$$= -\iota \langle n| [e^{\iota Ht} x e^{-\iota Ht} p(0) - p(0) e^{\iota Ht} x e^{-\iota Ht}] |m\rangle \tag{221}$$

$$= \sum_k -\iota[\langle n| [e^{\iota Ht} x e^{-\iota Ht} |k\rangle \langle k| p(0) |m\rangle - \langle n| p(0) |k\rangle \langle k| e^{\iota Ht} x e^{-\iota Ht}] |m\rangle] \tag{222}$$

$$= \sum_k -\iota[e^{\iota E_{nt}} \langle n| x |k\rangle e^{-\iota E_{kt}} \langle k| p(0) |m\rangle - \langle n| p(0) |k\rangle e^{\iota E_{kt}} \langle k| x |m\rangle e^{-\iota E_{mt}}] \tag{223}$$

We get,

$$b_{nm}(t) = -\iota \sum_k [e^{\iota E_{nk} t} x_{nk} p_{km} - e^{\iota E_{km} t} p_{nk} x_{km}] \tag{224}$$

where $E_{nk} = E_n - E_k$ and $E_{km} = E_k - E_m$.

When the Hamiltonian is of the form(CHO Hamiltonian):

$$H = \sum_{i=1}^{N} {P_i}^2 + U(x_1, x_2....x_N) \tag{225}$$

Calculating $[H, x]$,

$$[H, x] = [p^2, x] + [U(x_1, x_2....x_n), x] \tag{226}$$

$$= -2\iota p \tag{227}$$

The second part goes to zero. Now finding matrix element $\langle m| [H, x] |n\rangle$,

$$\langle m| Hx |n\rangle - \langle m| xH |n\rangle = -2\iota \langle m| p |n\rangle \tag{228}$$

$$E_m \langle m| x |n\rangle - E_n \langle m| x |n\rangle = -2\iota p_{mn} \tag{229}$$

$$E_{mn} x_{mn} = -2\iota p_{mn} \tag{230}$$

$$\therefore p_{mn} = \frac{\iota}{2} E_{mn} x_{mn} \tag{231}$$

Putting the value of 231 in 224, we get

$$b_{mn}(t) = -\iota \sum_k [e^{\iota E_n t} x_{nk} (\frac{\iota}{2} E_{km} x_{km}) - e^{\iota E_{km} t} (\frac{\iota}{2} E_{nk} x_{nk}) x_{km}] \tag{232}$$

$$\therefore \boxed{b_{nm}(t) = \frac{1}{2} \sum_k [x_{nk} x_{km} (E_{km} e^{\iota E_{nk} t} - E_{nk} e^{\iota E_{km} t})]} \tag{233}$$

where x_{nk} is the matrix element of x and E_{km} is the energy spectrum E_n.

With these, OTOCs can be numerically evaluated, following the below steps:

1. Solve the Schrödinger equation of the given system to obtain the energy eigenvalues and the wave functions.

2. Compute $x_{nm} = \langle n| x |m\rangle$ with numerical integration.

3. Substitute the result of step:2 to (233) to calculate $b_{nm}(t)$.

4. Evaluate the microcanonical OTOC $c_n(t)$ by substituting the result of step:3 to (219).

5. Evaluate the thermal OTOC $C_T(t)$ by using (217).

In these numerical evaluations, approximations by introducing a finite cut-off to the infinite sums are necessary. In the next section, we shall use this strategy to numerically evaluate the OTOCs in the CHO system.

12.3 OTOC for Harmonic Oscillator

Writing x and p in terms of lowering and raising operators,

$$x = \sqrt{\frac{\hbar}{2mw}}(a + a^{\dagger}) \tag{234}$$

$$p = \iota\sqrt{\frac{\hbar mw}{2}}(a - a^{\dagger}) \tag{235}$$

Now writing matrix element of x,

$$x_{nm} = \langle n| x |m\rangle \tag{236}$$

$$= \langle n| \sqrt{\frac{\hbar}{2mw}}(a + a^{\dagger}) |m\rangle \tag{237}$$

Taking all the standard symbols in natural units we have,

$$x_{nm} = \sqrt{\frac{1}{w}} \langle n| (a + a^{\dagger}) |m\rangle \tag{238}$$

$$= \sqrt{\frac{1}{w}}[\sqrt{m} \langle n|m-1\rangle + \sqrt{m+1} \langle n|m+1\rangle] \tag{239}$$

$$\tag{240}$$

Therefore, x_{nm} can be obtained as:

$$\boxed{x_{nm} = \sqrt{\frac{1}{w}}[\sqrt{m} \quad \delta_{n,m-1} + \sqrt{m+1} \quad \delta_{n,m+1}]} \tag{241}$$

Putting 241 in 233, we obtain:

$$b_{nm} = \frac{1}{2}\sum_k [\sqrt{\frac{1}{w}}(\sqrt{k} \quad \delta_{n,k-1} + \sqrt{k+1} \quad \delta_{n,k+1}).\sqrt{\frac{1}{w}}(\sqrt{m} \quad \delta_{k,m-1} + \sqrt{m+1} \quad \delta_{k,m+1}) [(E_{km}e^{\iota E_{nk}t} - E_{nk}e^{\iota E_{km}t})]] \tag{242}$$

b_{nm} can be obtained as:

$$b_{nm} = \delta_{nm} coswt \tag{243}$$

Calculating Microcanonical OTOC by using 219 is

$$c_n(t) = cos^2 wt \tag{244}$$

Calculating $C_T(t)$ using (217), we get,

$$C_T(t) = cos^2 wt \tag{245}$$

Hence, the OTOC of Harmonic Oscillator is coming out to be **Oscillatory**.

13 Exponential growth of thermal OTOC

Applying the techniques learnt from previous section, the variation of energy eigenvalues with n must be like,

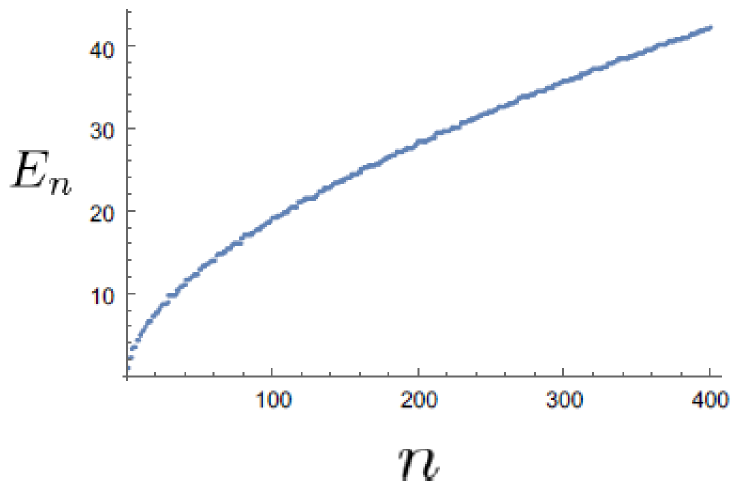


Figure 12: Energy eigenvalues of the CHO Hamiltonian with $\omega = 1$ and $g_0 = 0.1$.

13.1 Preparations: Microcanonical OTOC

To find the Microcanonical OTOC, first we need to solve the time-independent Schrödinger equation and obtain the energy eigenvalues and the wave functions

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi_n(x,y) + \left[\frac{\omega^2}{4}\left(x^2 + y^2\right) + g_0 x^2 y^2\right]\psi_n(x,y) = E_n\psi_n(x,y) \tag{246}$$

The energy levels are shown in the fig.13. We use package NDEigensystem to get eigenvalues in Mathematica Software. Using these solution we can compute the

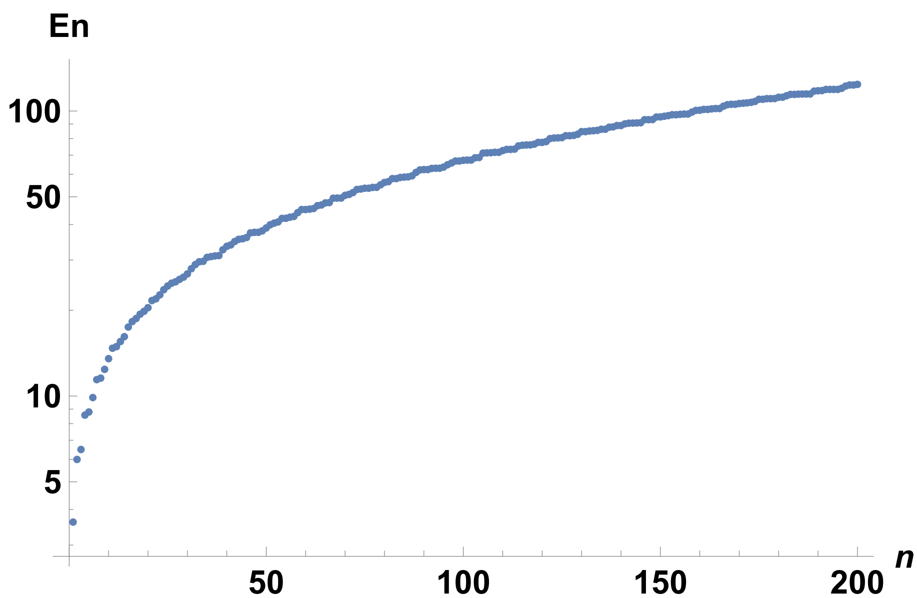


Figure 13: Variation of Energy eigenvalues of the CHO Hamiltonian with $\omega = 1$ and g_0=0.1

Microcanonical OTOC. We have shown the microcanonical OTOC computed numerically in fig.14.

For low modes, the microcanonical OTOC oscillates almost periodically and does not show any exponential growth. This characteristic is similar to the microcanonical OTOC of a harmonic oscillator.

On the other hand, the characteristics of the microcanonical OTOC deviates from that of the harmonic oscillator at higher modes. which was expected from the expression of $U(x, y)$.

The potential is well approximated (at low energy) by a harmonic oscillator around the origin , so the wave functions localized around the origin behave like that of the harmonic oscillator while for the higher modes, the the wave functions spread because the potential contributes dominantly.

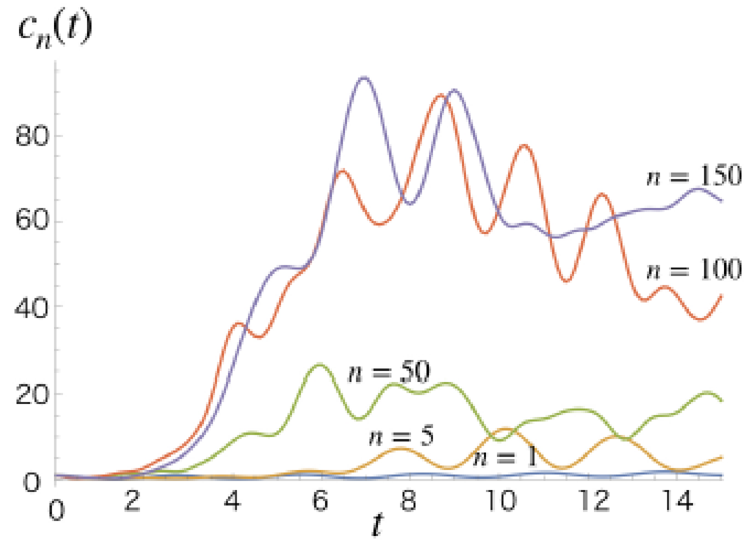


Figure 14: Microcanonical OTOC of the CHO Hamiltonian with $\omega = 1$ and g_0 =0.1.

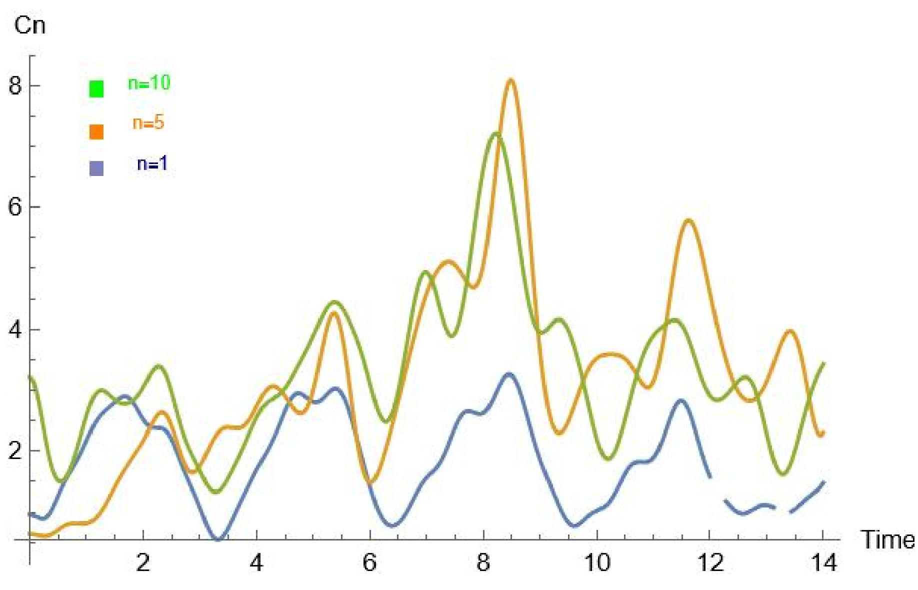


Figure 15: Microcanonical OTOC of the CHO Hamiltonian with $\omega = 1$ and g_0 =0.1.

14 Thermal OTOC

By substituting the numerical results of the microcanonical OTOC cn(t) to the expression 217 , we compute the thermal OTOC $C_T(t)$. The numerical results are shown in Fig below:

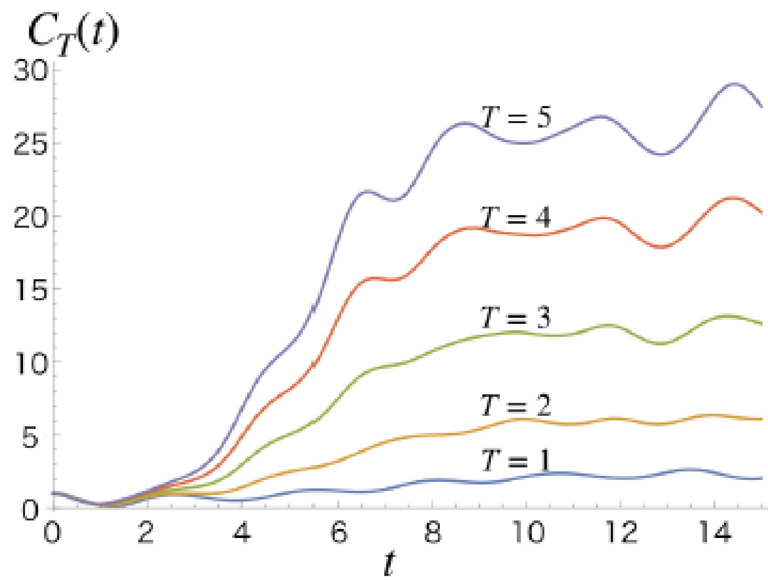


Figure 16: Thermal OTOC of the CHO Hamiltonian with $\omega = 1$ and $g_0 = 0.1$.

The obtained thermal OTOC shows two apparent characteristics: at the early time stage it grows, and at the late time stage it saturates to a constant value.

15 Anharmonic Oscillator

Consider the potential of an Anharmonic Oscillator,

$$U(x) = \frac{g_0}{4}x^4 \tag{247}$$

Now, for this potential , the schrodinger equation will be

$$-\frac{\partial^2\psi_n(x)}{\partial x^2} + \frac{1}{2}x^2\psi_n(x) + 0.1x^4\psi(x) = E_n\psi_n(x) \tag{248}$$

Form this equation we can get the Energy eigenvalues (energy levels are given in figure below) and the Wavefunction for the Anharmonic oscillator using NDEigensystem package of Mathematica software.

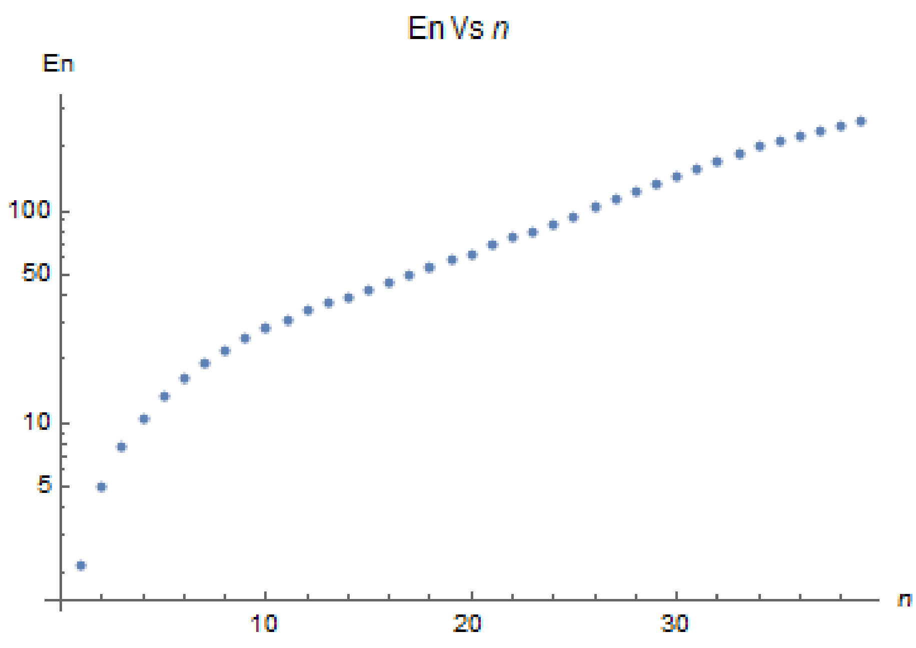


Figure 17: Energy eigenvalues of the Anharmonic Oscillator Hamiltonian with $\omega = 1$ and $g_0 = 0.1$.

Now, by applying the techniques learnt in previous section, we can compute the Microcanonical OTOC for the Anharmonic Oscillator analytically by using Laguerre Coefficients and WKB approximation [1].

Here, we have plotted the approximate behavior of microcanonical OTOC using Mathematica.

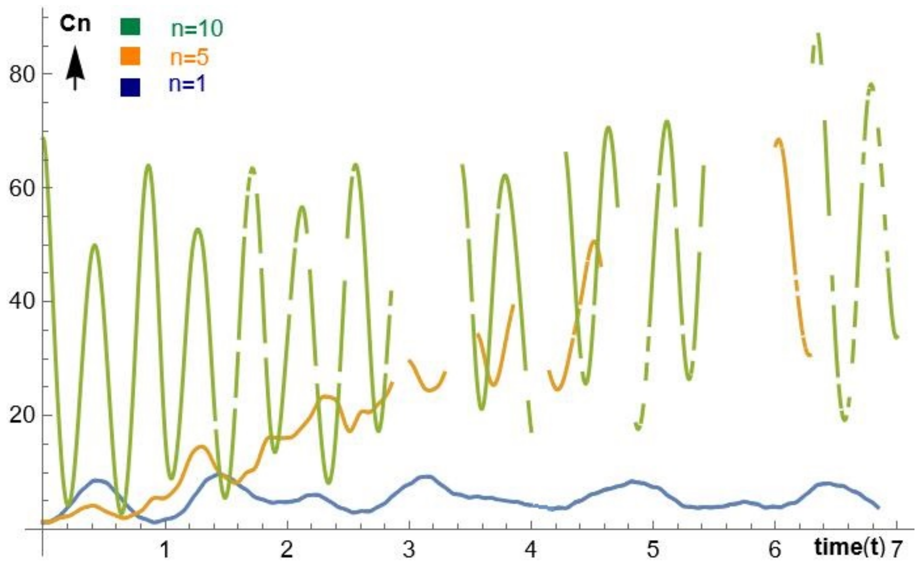


Figure 18: Microcanonical OTOC for Anharmonic Oscillator.

16 Conclusion

Looking at the limitations of Quantum Mechanics, We have seen that neither Quantum Mechanics nor its relativistic extension with Klein Gordon and Dirac equation can describe many particle systems. Although after applying field approach to our theory, we are able to deal with these shortcomings. Quantum Field theory is helpful in removing the shortcomings of Quantum Mechanics and providing results which are consistent with Special Relativity. It is the most fundamental theory which can help us provide an explanation to various phenomenons taking place in the Universe, like, particle creation and annihilation, intrinsic angular momentum (spin), magnetic moments, the fine structure properties of matter,etc. For explaining processes such as Scattering, QFT is a significant theory to describe particles with large degrees of freedom. The interaction between particles in complicated systems are described by interaction term present in the Lagrangian involving their corresponding quantum fields.These interaction can be visually represented by Feynman diagrams according to perturbation theory in quantum mechanics. The amplitudes $\mathcal{A}$ calculated using these diagrams can be further used to calculate scattering cross sections $\frac{d\sigma}{d\Omega} \propto |\mathcal{A}|^2$.

In the classical coupled harmonic oscillator system, at low energy, we are able to see the distinct orbits in the Poincaré section, so the system is in a **Regular phase**, while at high energy, orbits decay and the Poincaré section is filled with scattered points, meaning that the system is in a **Chaos phase**. In the quantum system, the thermal OTOC is more sensitive to the quantum chaos than the level statistics, and is able to discriminate the quantum chaos at lower energy (temperature). We calculated the OTOC for the very basic system of quantum field theory, harmonic oscillator which came out to be oscillatory in nature. At the end, another system (Anharmonic oscillator) was taken and we found that at low temperature, OTOCs are periodic, while at high temperature OTOCs exhibit rapid power-law growth followed by an apparent saturation consistent with the temperature-dependent value $2 < x^2 >_T < p^2 >_T$. In the same way , we can calculate OTOCs for various integrable and non-integrable example.[4]

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17 Future Scope and Objectives

So far we have had the basic understanding of Quantum Field theory and have studied about the role of Feynman Diagrams in interaction representation. We have also studied two chaotic systems and looked at the thermal OTOC as an indicator of its chaotic behavior. While the present study was performed for coupled harmonic oscillator and quartic oscillator potential, all of the steps presented here can be repeated for potentials $V(x) = x^N$ with arbitrary (even non-integer) N. We can also apply various approximation techniques to reduce instability in the graph of microcanonical OTOCs one of which has been described in [9].

We expect that some harmonic oscillator couplings other than we discussed in this paper will produce quantum chaos similarly, with different scaling properties. Studying the thermal OTOCs and scrambling timescales in systems given by some limits of coupled harmonic oscillators will lead the way to examine quantum gravity nature of matters explicitly.

18 Appendices

18.1 Maple Code for plotting Poincare Sections

In this code , the value of energy is changed and all the four plots of fig.(11) is obtained.

```
> restart
> with(DEtools, poincare, generate_ic, zoom, hamilton_eqs) :
> H := 1/2 (p1^2 + p2^2 + q1^2 + q2^2) + 0.05 q1^2 q2^2
        H := 1/2 p1^2 + 1/2 p2^2 + 1/2 q1^2 + 1/2 q2^2 + 0.05 q1^2 q2^2                                   (1)
> H, t = -1500 ..1500, {[0, 0.1, 0.2, 0.2, 0]};
        1/2 p1^2 + 1/2 p2^2 + 1/2 q1^2 + 1/2 q2^2 + 0.05 q1^2 q2^2, t = -1500 ..1500, {[0, 0.1, 0.2, 0.2, 0]}  (2)
> ics := generate_ic(H, {t = 0, p1 = 1, q1 = 2, q2 = 0, energy = 20}, 9)
        ics := {[0., 1., 5.916079783, 2., 0.]}                                                            (3)
> ic1 := generate_ic(H, {t = 0, p1 = 1, q1 = 2, q2 = 0, energy = 20}, 1)
        ic1 := {[0., 1., 5.916079783, 2., 0.]}                                                            (4)
> ic2 := generate_ic(H, {t = 0, p1 = 2, q1 = 2, q2 = 0, energy = 20}, 1)
        ic2 := {[0., 2., 5.656854249, 2., 0.]}                                                            (5)
> ic3 := generate_ic(H, {t = 0, p1 = 2, q1 = 2, q2 = 2, energy = 20}, 1)
        ic3 := {[0., 2., 5.138093031, 2., 2.]}                                                            (6)
> ic4 := generate_ic(H, {t = 0, p1 = 1.5, q1 = 2, q2 = 3, energy = 20}, 1)
        ic4 := {[0., 1.5, 4.598912915, 2., 3.]}                                                           (7)
> ic5 := generate_ic(H, {t = 0, p1 = 1, q1 = 1, q2 = 4, energy = 20}, 1)
        ic5 := {[0., 1., 4.516635916, 1., 4.]}                                                            (8)
```

```
> ic6 := generate_ic(H, {t = 0, p2 = 1, q1 = 1, q2 = 1, energy = 20}, 1)
        ic6 := {[0., 6.074537019, 1., 1., 1.]}                                                            (9)
> ic7 := generate_ic(H, {t = 0, p2 = 0.5, q1 = 1, q2 = 1, energy = 20}, 1)
        ic7 := {[0., 6.135959583, 0.5, 1., 1.]}                                                           (10)
> ic8 := generate_ic(H, {t = 0, p2 = 0.7, q1 = 1, q2 = 1, energy = 20}, 1)
        ic8 := {[0., 6.116371473, 0.7, 1., 1.]}                                                           (11)
> ic9 := generate_ic(H, {t = 0, p2 = 0.3, q1 = 1, q2 = 0.5, energy = 20}, 1)
        ic9 := {[0., 6.215705913, 0.3, 1., 0.5]}                                                          (12)
> ics := ic1 ∪ ic2 ∪ ic3 ∪ ic4 ∪ ic5 ∪ ic6 ∪ic7 ∪ ic8∪ ic9
ics := {[0., 1., 4.516635916, 1., 4.], [0., 1., 5.916079783, 2., 0.], [0., 1.5, 4.598912915, 2., 3.], [0., 2., 5.138093031, 2., 2.], [0., 2., 5.656854249, 2., 0.], [0., 6.074537019, 1., 1., 1.], [0.,   (13)
    6.116371473, 0.7, 1., 1.], [0., 6.135959583, 0.5, 1., 1.], [0., 6.215705913, 0.3, 1., 0.5]}
> poincare(H, t = -2000 ..2000, ics, stepsize = 0.1, iterations = 3, scene = [q2, p2])
```

18.2 Mathematica code for plotting Energy Eigenvalues

In this code, we will replace the hamiltonian by that given in eq.248 to get fig.17

```
In[ ]:= {val, func} = NDEigensystem[{-Laplacian[u[x, y], {x, y}] + 0.25 (x^2 + y^2) u[x, y] + 0.1 x^2 y^2 u[x, y], DirichletCondition[u[x, y] == 0, True]},
          u[x, y], {x, 0, 5}, {y, 0, 5}, 200, Method → {"Interpolation" → {"ExtrapolationHandler" → {(Indeterminate &), "WarningMessage" → False}}}];

In[ ]:= ListLogPlot[val, AxesLabel → {n, E_n}]

In[ ]:= Show[%3, AxesLabel → {n, HoldForm[En]}, PlotLabel → None, LabelStyle → {FontFamily → "Arial", 13, GrayLevel[0], Bold}]
```

18.3 Mathematica Code for plotting Microcanonical OTOC

We replace the hamiltonian by that given in eq.248 to get fig.18

```
In[ ]:= {val, func} = NDEigensystem[-Laplacian[u[x, y], {x, y}] + 0.25 (x^2 + y^2) u[x, y] + 0.1 x^2 y^2 u[x, y], u[x, y], {x, 0, 5}, {y, 0, 5}, 12];

In[ ]:= expct = Table[0, 10, 10];
        engdif = Table[0, 10, 10];

In[ ]:= For[a = 1, a < 11, a++,
          For[b = 1, b < 11, b++,
            Needs["FunctionApproximations`"];
            expct[[a, b]] = NIntegrateInterpolatingFunction[(func[[a]])*x (func[[b]]), {x, 0, 5}, {y, 0, 5}];
            engdif[[a, b]] = val[[a]] - val[[b]]; ]; ];

In[ ]:= btrans = Table[0, 1, 10];
        For[d = 1, d < 11, d++,
          btrans[[1, d]] = 1/2 Sum[(expct[[10, e]]) × (expct[[e, d]]) × (engdif[[e, d]] × Exp[ⅈ (engdif[[10, e]]) t] - (engdif[[10, e]]) × (Exp[ⅈ (engdif[[e, d]]) t])), {e, 1, 10}];];
        cten[t_] := Sum[btrans[[1, f]] × (btrans[[1, f]])*, {f, 1, 10}];

In[ ]:= cten[t]
```

```
In[ ]:= rcten[t_] :=
  … 16 725 … +
  ⅈ (0.00006055191385565911` + 0.` ⅈ) Cos[(0.` + 0.` ⅈ) - 8.526075541443184` Re[t]] × Cos[(0.` + 0.` ⅈ) + 29.164307110455212` Re[t]] × Sin[(0.` + 0.` ⅈ) - 37.690382651898396` Re[t]] +
    0.00008180655387306647` e^(0.` - (0.` + 2.149937072013259` ⅈ) (t - Re[t])) Cos[(0.` + 0.` ⅈ) - 6.376138469429925` Re[t]] × Cos[(0.` + 0.` ⅈ) + 29.164307110455212` Re[t]] ×
    Sin[(0.` + 0.` ⅈ) - 37.690382651898396` Re[t]] + … 15 596 … )
  large output | show less | show more | show all | set size limit...

In[ ]:= rcone[t_] :=
  -0.0028481813485730506` e^(0.` - (0.` + 8.526075541443184` ⅈ) (t - Re[t])) Cos[(0.` + 0.` ⅈ) - 45.42043569052018` Re[t]] × Cos[(0.` + 0.` ⅈ) + 36.894360149076995` Re[t]] +
  0.00008180655387306645` e^(0.` - (0.` + 2.149937072013259` ⅈ) (t - Re[t])) Cos[(0.` + 0.` ⅈ) - 45.42043569052018` Re[t]] × Cos[(0.` + 0.` ⅈ) - 6.376138469429925` Re[t]] ×
  Cos[(0.` + 0.` ⅈ) + 36.894360149076995` Re[t]] + … 17 255 … + (0.0005223773832309857` + 0.` ⅈ) … 3 … Sin[… 1 …] +
  ⅈ
  (… 16 220 … + (0.0005223773832309857` + 0.` ⅈ) e^(0.` - (0.` + 7.877782313238072` ⅈ) (t - Re[t])) Sin[(0.` + 0.` ⅈ) - 68.20860433154546` Re[t]] × Sin[(0.` + 0.` ⅈ) + 7.877782313238072` Re[t]] ×
    Sin[(0.` + 0.` ⅈ) + 68.20860433154546` Re[t]])
  large output | show less | show more | show all | set size limit...

In[ ]:= rcfive[t_] :=
  -0.007303416608720521` e^(0.` - (0.` + 4.1523144425211544` ⅈ) (t - Re[t])) Cos[(0.` + 0.` ⅈ) - 12.491330174453434` Re[t]] × Cos[(0.` + 0.` ⅈ) + 8.33901573193228` Re[t]] + … 17 325 … +
  ⅈ (0.0006154189250802065` e^(0.` - (0.` + 8.526075541443184` ⅈ) (t - Re[t])) Cos[(0.` + 0.` ⅈ) + 33.35100839986634` Re[t]] × Sin[(0.` + 0.` ⅈ) - 41.87708394130952` Re[t]] + … 16 853 … )
  large output | show less | show more | show all | set size limit...

In[ ]:= Plot[{rcone[t], rcfive[t], rcten[t]}, {t, 0, 14}]

In[ ]:= Show[%40, AxesLabel → {HoldForm[Time], HoldForm[Cn]}, PlotLabel → None, LabelStyle → {GrayLevel[0]}]
```

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