Space-Time Dynamics in Open and Closed Quantum Systems

by

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Certificate

It is certified that the research work in this thesis entitled **Space-Time Dynamics in Open and Closed Quantum Systems** has been carried out and completed by **Muhammad Hashim, Reg. No. 02182111007** is accepted in its present form by the Department of Physics, Quaid-iAzam University, Islamabad, as satisfying the dissertation requirement for the degree of Master of Philosophy in Physics

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Abstract

A fundamental feature of the physics of waves is interference. The formation of highly regular spatio-temporal patterns in the quantum mechanical probability density of confined particles is a striking example. The density distributions have been termed "quantum interference patterns". In this thesis we track down the dynamics of open and closed quantum systems in space and time. For this purpose we construct the initial wave packet and investigate how it evolves in time for such quantum systems. We introduce the concept of quantum revivals which are characterized by initially localized quantum states that have a short-term, quasi-classical time evolution, which then can spread significantly over several orbits, only to reform later in the form of a quantum revival where the spreading reverses itself, the wave packet relocalizes, and the semi-classical periodicity is once again evident. Relocalization of the initial wave packet into a number of smaller copies of the initial packet ('minipackets' or 'clones') is also possible, giving rise to fractional revivals. Systems exhibiting such behavior are a fundamental realization of time-dependent interference phenomena for bound states with quantized energies in quantum mechanics and are therefore of wide interest in the physics community. We Introduce the concept of autocorrelation function, that measures the overlap (in Hilbert space) of a time-dependent quantum mechanical wave function, with its initial value. The explicit expression for the autocorrelation function for the time-dependent Gaussian solution of the Schrodinger equation, in the case of a particle in a box, is evaluated.

Contents

List of Figures

Chapter 1

Introduction

Study of time development of localized systems in quantum mechanics has been the interest of both researchers and student of the subject since it's early days. Schrodinger, Pauli, Dirac and other pioneers of the subject analyzed basic bounded systems for both conceptual and philosophical development of the subject. Among those basic bounded systems particle in a box is one of the most fundamental and exactly solvable system. In this thesis we discuss the quantum dynamics of such systems.

1.1 Diffraction

In general, diffraction happens when waves hit an obstruction or aperture. The obstruction or aperture must have a similar size scale to the wave's wavelength. In classical physics, diffraction happens when waves diverge from small gaps or bend around obstructions. In quantum physics, diffraction also happens when matter exhibits wavelike characteristics. Thomas Young's double-slit experiment is a significant historical illustration of diffraction. In this early 1800s experiment, Young directed sunlight through two small openings as depicted in Figure (1.1). Interference is the term used to describe the interaction of waves when light passes through the first single slit and subsequently the second double slit. Diffraction is what causes the maxima and minima pattern on the screen. The first piece of experimental evidence to undermine the widely held Newtonian notion that light is made up of

particles was this result. Instead, light acted like a wave, as demonstrated by the maxima and minima pattern. Later, studies conducted in the 20th century using similar diffraction and interference techniques demonstrated that both matter and light may behave like waves.

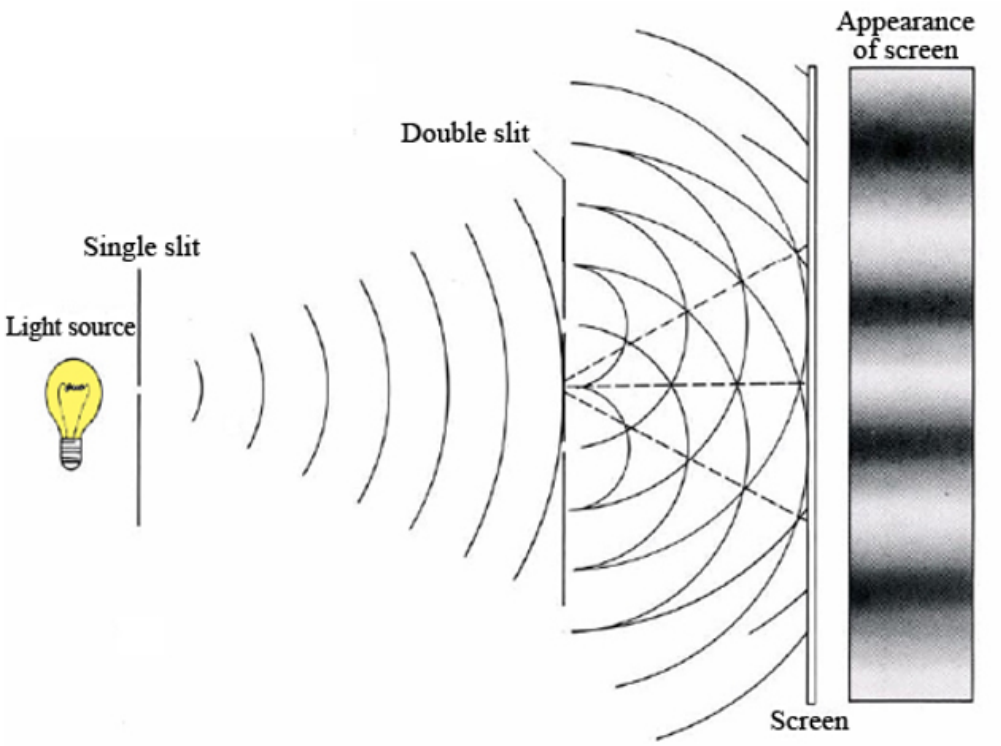

Figure 1.1: A schematic of Thomas Young's double slit experiment [1].

1.1.1 Near-Field Versus Far-Field Diffraction

In optics, diffraction behavior is classified by whether it occurs in the near-field or the far-field. The near-field is close to an aperture where the wavefront curvature is important. The far-field is farther away from an aperture where the wavefronts can be estimated as parallel. Diffraction that occurs in the far-field is called Fraunhofer diffraction and diffraction that occurs in the near-field is called Fresnel diffraction. Formally, Fraunhofer diffraction occurs when,

$$\frac{a^2}{L\lambda} \ll 1 \qquad \text{(A)}$$

and Fresnel diffraction occurs when,

$$\frac{a^2}{L\lambda} \gg 1 \tag{B}$$

where a is the aperture or slit size, L is the distance from aperture, and λ is the wavelength of light[2]. Young's double slit experiment is an example of far-field diffraction. Meanwhile, the Talbot effect occurs in the near-field. In the near-field, Fresnel approximations are made and the wavefront curvature cannot be ignored.

1.2 Quantum Interference

Quantum interference is a phenomenon that occurs when two or more quantum states combine, producing a new quantum state that exhibits characteristics that are not present in the individual states. This phenomenon is a consequence of the wave-like nature of quantum particles, which allows them to interfere with each other just as waves in classical physics can interfere with each other. In quantum mechanics, particles such as electrons and photons can be described as wave-particle dualities, meaning that they can exhibit both wave-like and particle-like behavior. When two or more of these particles are combined, their wave functions can interfere with each other, producing patterns of constructive and destructive interference. These patterns can be observed through experiments such as the double-slit experiment, in which a beam of particles is directed through two closely spaced slits and the resulting interference pattern is observed on a detector screen. Quantum interference has many important implications in various fields of physics and technology, including quantum computing, quantum cryptography, and the study of quantum systems.

1.2.1 Quantum Interference Patterns

Quantum interference patterns are patterns that arise when two or more waves overlap and interfere with each other. In quantum mechanics, these patterns can occur when two or more quantum states are superimposed,

resulting in the creation of an interference pattern that reflects the relative phase differences between the states. One of the most famous examples of quantum interference patterns is the double-slit experiment, in which a beam of particles is passed through two slits and strikes a screen on the other side. When a single particle is sent through the slits, it will create a simple pattern on the screen, with two bright spots corresponding to the locations of the slits. However, if many particles are sent through the slits at the same time, an interference pattern will be created on the screen, with alternating bright and dark regions that reflect the quantum superposition of the particles as they pass through the slits. Quantum interference patterns are important because they demonstrate the wave-like nature of quantum particles, as well as their ability to exhibit both particle-like and wave-like behaviors simultaneously. They also have practical applications in fields such as quantum computing, where they are used to manipulate the quantum states of particles in order to perform certain calculations.

1.3 Quantum Systems

Quantum systems are physical systems that are described using the principles of quantum mechanics. Quantum mechanics is a fundamental theory of physics that describes the behavior of matter and energy at the atomic and subatomic scales, and it is based on the principles of wave-particle duality and quantum superposition. In a quantum system, the state of the system can be described using a wave function, which is a mathematical function that describes the probability of finding the system in a particular state. The wave function evolves according to the principles of quantum mechanics, which govern the behavior of quantum systems. Quantum systems are characterized by several unique properties that are not observed in classical systems, such as wave-particle duality, quantum superposition, and quantum entanglement. These properties have important implications for the behavior and evolution of quantum systems, and they have been the subject of much research and study in the field of quantum mechanics. Quantum systems have important applications in a variety of fields, including quantum computing, quantum communication, quantum sensing, and quantum thermodynamics.

Understanding the behavior of quantum systems and the principles that govern them is essential for the development of new technologies and advances in these fields.

1.3.1 Open Quantum Systems

Open quantum systems are quantum systems that interact with their environment or are subject to decoherence, which is the loss of coherence or the ability to maintain a superposition of states. These systems are not isolated from their environment and are affected by external influences, such as interactions with other systems or the presence of noise or other types of perturbations. Open quantum systems are described using density matrices, which are mathematical objects that describe the statistical properties of the system. Density matrices allow researchers to track the evolution of the system over time and to study the effects of external perturbations on the system. Open quantum systems are an important concept in quantum mechanics, as they provide a framework for understanding the behavior of quantum systems that are not isolated from their environment. Understanding the properties and behavior of open quantum systems can be helpful in the development of more efficient and reliable quantum algorithms and protocols, as well as in improving the accuracy and precision of quantum sensors and measurement devices.

1.3.2 Closed Quantum Systems

A closed quantum system is a system that is isolated from its environment and is therefore not subject to decoherence or other types of interactions. These systems are described using wave functions, which describe the probability of finding the system in a particular state. In a closed quantum system, the wave function evolves according to the principles of quantum mechanics and is not affected by external influences. Closed quantum systems are characterized by their ability to maintain quantum coherence, which is the ability to maintain a superposition of states or the ability to exist in multiple states simultaneously. This property is essential for certain types of quantum applications, such as quantum computing and quantum simulation, which require

high levels of quantum coherence in order to perform complex quantum operations or simulate the behavior of other quantum systems. Closed quantum systems are an important concept in quantum mechanics, as they provide a framework for understanding the behavior of quantum systems that are isolated from their environment. They have important applications in a variety of fields, including quantum computing, quantum simulation, and quantum metrology. Understanding the properties and behavior of closed quantum systems is essential for the development of new technologies and advances in these fields, and it can help researchers and scientists develop more efficient and reliable quantum algorithms and protocols, as well as improve the accuracy and precision of quantum sensors and measurement devices.

1.4 Revivals

A revival refers to the phenomenon of a system returning to a state that is similar to its initial state at regular intervals. This can happen in both classical and quantum systems when the system is subjected to certain types of time-dependent perturbations, such as periodic or quasi-periodic driving forces. One example of revivals in classical physics is the periodic oscillations of a simple harmonic oscillator, such as a mass on a spring or a pendulum. In these cases, the system returns to its initial state at regular intervals due to the influence of external forces, such as the restoring force of a spring or the force of gravity. In quantum physics, revivals can occur in certain types of quantum systems when they are subject to periodic or quasi-periodic perturbations. One example of this is the Rabi oscillation, which occurs in a system of two energy levels when the system is subjected to a periodic driving force. In this case, the system periodically oscillates between the two energy levels, returning to its initial state at regular intervals.

1.4.1 Importance of Quantum Revivals:

Quantum revivals are an important phenomenon in the field of quantum mechanics, as they provide insight into the fundamental nature of quantum systems and the role of time and measurement in the quantum world. One

important aspect of quantum revivals is that they demonstrate the wave-like nature of quantum systems. When a quantum system exhibits quantum revivals, it is a clear indication that the system is behaving like a wave, rather than a classical object. This helps to confirm our understanding of the quantum world and the principles that govern it. In addition, quantum revivals can be used to study the behavior of quantum systems under different conditions, such as when they are subjected to periodic or quasi-periodic perturbations. This can help researchers gain a better understanding of how quantum systems respond to external influences and how they evolve over time.

1.5 This Thesis

This thesis seeks to our understanding of the revival of wave packets in a one-dimensional box by exploring the role of the autocorrelation function in this process. In this context firstly, I will elucidate the wave packets dynamics in chapter-2. In which we will discuss general features of the motion of a wave-packet and see how it changes shape. Moreover, I will demonstrate the construction of Gaussian wave packet and will develop a model for many Gaussians which would be helpful in the study of open and closed quantum systems. Secondly, I will provide background materials for development of mathematical model that will help us in observing the revival phenomena. Thirdly, I will track down the discussions about quantum revivals by introducing the concept of autocorrelation function in chapter-4. In addition we will investigate the quantum dynamics of open and closed quantum systems. Finally, I will conclude my thesis.

Chapter 2

Wave Packet Dynamics

In this chapter we will develop concepts of wave packets. It is a key tool for understanding the behavior of quantum systems. The dynamics of quantum systems can be studied by introducing Gaussian wave packets. In this chapter we will see how an initial Gaussian wave packet can be constructed mathematically. In addition we will discuss the integral operation, Fourier transform and time evolution of Gaussian wave packet.

2.1 Wave Packet in Quantum Mechanics

In quantum mechanics, a wave packet is a mathematical function that describes the behavior of a particle or system of particles. It is a combination of multiple waves with different wavelengths and amplitudes, and it can be used to represent the probability of finding a particle at a particular location at a given time. The concept of a wave packet is important because it helps us understand how particles behave in quantum systems. For example, the wave packet of an electron in an atom describes the probability of finding the electron at a particular energy level within the atom. Similarly, the wave packet of a particle in a box describes the probability of finding the particle within the boundaries of the box. Wave packets are often described using the mathematical concept of a wave function, which is a function that describes the probability amplitude of a particle at a particular location and time. The wave function is related to the wave packet through the Heisenberg

uncertainty principle, which states that the more accurately we know the position of a particle, the less accurately we can know its momentum, and vice versa. This uncertainty is due to the wave-like nature of particles in quantum systems, and it is a fundamental aspect of quantum mechanics.

2.1.1 Characteristics of Wave Packets

Here are some characteristics of wave packets in quantum mechanics:

- Wave packets are described using wave functions: A wave function is a mathematical function that describes the probability amplitude of finding a particle at a particular location and time. It is related to the wave packet through the Heisenberg uncertainty principle.
- Wave packets are used to represent the probability of finding a particle at a particular location: The wave packet of a particle is a mathematical function that describes the probability of finding the particle at a particular location at a given time. This probability is represented by the probability amplitude of the wave function.
- Wave packets are characterized by their width and energy: The width of a wave packet is a measure of how spread out it is in space, and it is related to the uncertainty in the position of the particle. The energy of a wave packet is a measure of the particle's kinetic energy, and it is related to the uncertainty in the momentum of the particle.
- Wave packets can exhibit wave-like behavior: Particles in quantum systems can exhibit both wave-like and particle-like behavior. The wave-like nature of particles is related to the wave packet through the wave function, which describes the probability amplitude of the particle at a particular location and time.
- Wave packets can be used to study various phenomena in quantum systems: Wave packets are a useful tool for understanding the behavior of particles in quantum systems, and they are often used to study phenomena such as quantum tunneling, quantum coherence, and the behavior of particles in quantum wells and quantum dots.

2.1.2 Mathematical Interpretation

A wavepacket is a superposition of plane waves e^{ikx} with various wavelengths. Where k is the wave number related to the wavelength through $k = 2\pi/\lambda$. Consider a wavepacket at $t = 0$ of the form:

$$w(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mu(k) e^{ikx} dk \tag{2.0.A}$$

If we know $w(x,0)$ then $\mu(k)$ is calculable. In fact, by the Fourier inversion theorem, the function $\mu(k)$ is the Fourier transform of $w(x,0)$, so we can write

$$\mu(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} w(x,0) e^{-ikx} dx. \tag{2.0.B}$$

There is symmetry in these two equations. So, we can check that how the uncertainties in $w(x,0)$ and $\mu(k)$ are related. In the quantum mechanical interpretation of the these equations, a plane wave with momentum $\hbar k$ is of the form e^{ikx}. Thus the Fourier representation of the wave $w(x,0)$ gives a way to represent the wave as a superposition of plane waves of different momenta. In our case $w(x,0)$ is not real. We can show that $w(x,0)$ is real if and only if $\mu^*(-k) = \mu(k)$. By complex conjugating the eqn.(2.0.A) for $w(x,0)$:

$$w^*(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mu^*(k) e^{-ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mu^*(-k) e^{ikx} dk. \tag{2.1}$$

In the second step we let $k \to -k$ in the integral, which is allowable because we are integrating over all k, and the two sign flips, one from the dk and one from switching the limits of integration, cancel each other out. If $\mu^*(-k) = \mu(k)$ then

$$w^*(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mu(k) e^{ikx} dk = w(x,0) \tag{2.2}$$

as we wanted to check. If, on the other hand we know that $w(x,0)$ is real then the equality of w^* and w gives,

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mu^*(-k) e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mu(k) e^{ikx} dk \tag{2.3}$$

which is equivalent to

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\mu^*(-k) - \mu(k)\right) e^{ikx} dk = 0. \tag{2.4}$$

This equation actually means that object inside the brace must vanish. Indeed, the integral is computing the Fourier transform of the object with the brace, and it tells us that it is zero. But a function with zero Fourier transform must be zero itself (by the Fourier theorem). Therefore reality implies $\mu^*(-k) = \mu(k)$.

2.2 Gaussian Wave packet

A Gaussian wave packet is a type of wave packet that is characterized by a Gaussian probability distribution function. In other words, the probability of finding a particle at a particular location is described by a bell-shaped curve that follows a Gaussian distribution. Gaussian wave packets are often used to model the behavior of particles in quantum systems because they are relatively simple and easy to work with, mathematically. In quantum mechanics, a Gaussian wave packet can be described by a wave function of the form:

$$w(x,t) = Ae^{-\frac{x^2}{2L^2} + ikx - iEt/\hbar} \tag{2.5}$$

where A is the normalization constant, x is the position of the particle, L is the width of the wave packet, k is the wave vector, E is the energy of the particle, t is the time, and $\hbar$ is the reduced Planck constant. The wave function of a Gaussian wave packet is characterized by three parameters: the width of the wave packet (L), the wave vector (k), and the energy (E). These parameters can be used to control the behavior of the wave packet, such as its position, momentum, and uncertainty. In general, Gaussian wave packets are used to model the behavior of particles in quantum systems that are localized in space and have well-defined energy and momentum. They are often used to study phenomena such as quantum tunneling and quantum coherence, and they are a useful tool for understanding the behavior of particles in various quantum systems.

2.2.1 Initial Construction of the Gaussian Packet

To express the circumstance that "x-measurement (performed at time $t = 0$ with an instrument of imperfect resolution) has shown the particle to reside in the vicinity of the point $x = a$" we write $P(x,0) \equiv |w(x,0)|^2=$ [some properly positioned and shaped distribution function] and noticing that such a statement supplies only limited information about the structure of $w(x,0)$ itself

$$w(x,0) = \sqrt{P(x,0)}.e^{i\alpha(x,0)} \tag{2.6}$$

phase factor remains at present arbitrary.The phase factor has entered with simple innocence upon the stage, but is destined to play a leading role as the drama unfolds. Whether we proceed from some tentative sense of the operating characteristics of instruments of finite resolution or seek only to model such statements in a concrete but analytically tractable way, it becomes fairly natural to look to the special case given by,

$$P(x,0) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left[\frac{x-\alpha}{\sigma}\right]^2}. \tag{2.7}$$

The Gaussian on the right defines the "normal distribution" with mean; $< x >= a$, variance$\equiv$ (uncertainty)^2; $< (x-a)^2 >= \sigma^2$ and the associated wave function reads

$$w(x,0) = \left[\frac{1}{\sigma\sqrt{2\pi}}\right]^{\frac{1}{2}} e^{-\frac{1}{4}\left[\frac{x-\alpha}{\sigma}\right]^2}.e^{i\alpha(x,0)}. \tag{2.8}$$

Writing $w(x,0) \equiv (x|w)_0$ to draw attention to the fact that we're working in the x-representation.
Now we can accomplish the momentum representation as follows,

$$w(p,0) \equiv (p|w)_0 = \int (p|x)dx(x|w)_0 = \frac{1}{h}\int e^{-\frac{i}{\hbar}px} w(x,0)dx$$

$$= \frac{1}{h}\int e^{-\frac{i}{\hbar}px} w(x,0)dx \tag{2.9}$$

but cannot be carried out in detail until the phase factor has been specified[1] If, in the Gaussian case eqn.(2.8), we set α=0 then eqn.(2.9) gives

$$\mu(p,0) = \left[\frac{1}{\lambda\sqrt{2\pi}}\right]^{1/2} e^{-\frac{1}{4}\left[\frac{p}{\lambda}\right]^2}.e^{-\frac{i}{\hbar}\alpha p}, \tag{2.10}$$

with $\lambda \equiv \hbar/2\sigma$. Whence

$$Q(p) = \frac{1}{\lambda\sqrt{2\pi}} e^{-\frac{1}{2}\left[\frac{p}{\lambda}\right]^2}.e^{-\frac{i}{\hbar}\alpha p}, \tag{2.11}$$

which is again normal, but centered at the origin of p-space,
$< p >= 0$
$< (p-0)^2 >= \lambda^2$
In the relation

$$\sigma\lambda = \triangle x.\triangle p = \frac{1}{2}\hbar, \tag{2.12}$$

we have encountered an instance of optimal compliance with the Heisenberg uncertainty principle: $\triangle x.\triangle p \geq \frac{1}{2}\hbar$.
To achieve arbitrary placement of the origin of the normal distribution in momentum space i.e., to achieve,

$$eqn.(2.11) \rightarrow Q(p) = \frac{1}{\lambda\sqrt{2\pi}} e^{-\frac{1}{2}\left[\frac{p-b}{\lambda}\right]^2}, \tag{2.11}$$

it might appear most natural in place of eqn.(2.10) simply to write

$$\mu(p,0) = \left[\frac{1}{\lambda\sqrt{2\pi}}\right]^{1/2} e^{-\frac{1}{4}\left[\frac{p-b}{\lambda}\right]^2}.e^{-\frac{i}{\hbar}\alpha(p-b)}. \tag{2.12}$$

But then

$$w(x,0) = \frac{1}{\sqrt{h}} \int e^{\frac{i}{\hbar}px}\mu(p,0)dp. \tag{2.13}$$

[1]The statement
Normalization of $P(x,0) \equiv |w(x,0)|^2 \implies$ normalization of Q(p)$\equiv |\mu(p)|^2$ is, however, phase-insensitive, and is the upshot of Parseval's theorem: from P. Morse and H. Feshbach, Methods of Theoretical Physics (1953), p. 456.

Omitting the phase factor we get,

$$w(x,0) = \frac{1}{\sqrt{h}} \int e^{\frac{i}{\hbar}px} \left\{ \left[\frac{1}{\lambda\sqrt{2\pi}} \right]^{1/2} e^{-\frac{1}{4}\left[\frac{p-b}{\lambda}\right]^2} \right\} dp \tag{2.14}$$

$$= \left[\frac{1}{\sigma\sqrt{2\pi}} \right]^{1/2} e^{\frac{i}{\hbar}} e^{-\frac{i}{4}\left[\frac{x}{\sigma}\right]^2} bx \tag{2.15}$$

where,

$$\sigma \equiv \hbar/2\lambda. \tag{2.16}$$

The resulting distribution function,

$$P(x,0) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left[\frac{x}{\sigma}\right]^2}, \tag{2.17}$$

is again normal but centered at the origin in configuration space; it is precisely eqn.(2.7) with $a = 0$.

2.2.2 Integral of a Gaussian Function

Let, $f(x) = ae^{-bx^2}$ with $a > 0$ and $b > 0$. Noting that $f(x)$ is positive everywhere, the integral I of $f(x)$ over R for particular a and b is,

$$I = \int_{-\infty}^{+\infty} f(x)dx. \tag{2.18}$$

To solve this 1-dimensional integral, we will start by computing its square. By the separability property of the exponential function, it follows that we'll get a 2-dimensional integral over a 2-dimensional gaussian. If we can compute that, the integral is given by the positive square root of this integral.

$$I^2 = \int_{-\infty}^{+\infty} f(x)dx \int_{-\infty}^{+\infty} f(y)dy = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x)f(y)dydx \tag{2.19}$$

$$= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} ae^{-bx^2}ae^{-by^2}dydx \tag{2.20}$$

$$= a^2 \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-b(x^2+y^2)}dydx. \tag{2.21}$$

Now we will make a change of variables from (x, y) to polar coordinates (α,r). The determinant of the Jacobian of this transform is r. Therefore,

$$I^2 = a^2 \int_0^{2\pi} \int_0^{\infty} re^{-br^2} dr d\alpha \tag{2.22}$$

$$= \frac{a^2}{-2b} \int_0^{2\pi} \int_0^{\infty} e^{-br^2} dr d\alpha \tag{2.23}$$

$$= \frac{a^2}{-2b} \int_0^{2\pi} -1 d\alpha \tag{2.24}$$

$$I^2 = \frac{\pi a^2}{b}. \tag{2.25}$$

Taking the positive square root gives,

$$I = a\sqrt{\frac{\pi}{b}}. \tag{2.26}$$

Example

Requiring $f(x)$ to integrate to 1 over R gives the equation,

$$I = a\sqrt{\frac{\pi}{b}} = 1 \tag{2.27}$$

$$a = \sqrt{\frac{b}{\pi}}. \tag{2.28}$$

And substitution of,

$$b = \frac{1}{2\sigma^2}, \tag{2.29}$$

gives the Gaussian distribution $g(x)$ with zero mean and σ variance,

$$g(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}}. \tag{2.30}$$

2.2.3 The Fourier Transform of a Gaussian Function

Evaluating the bilateral Laplace transform $B(s)$ of $f(x)$ by using the intermediate result. The Fourier transform is then given by $F(w) = B(iw)$.

$$B(s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-sx} dx \tag{2.31}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a e^{bx^2} e^{-sx} dx \tag{2.32}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a e^{-(bx^2+sx)} dx. \tag{2.33}$$

Completing the square in the exponent,

$$b(x+k)^2 = bx^2 + 2bkx + bk^2. \tag{2.34}$$

By comparing factors of x we see that $2bk = s$ and thus $k = \frac{s}{2b}$. Now,

$$b(x + \frac{s}{2b})^2 - \frac{s^2}{4b} = bx^2 + sx \tag{2.35}$$

$$B(s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} a e^{-b\left(x+\frac{s}{2b}\right)^2 - \frac{s^2}{4b}} dx \tag{2.36}$$

$$B(s) = \frac{1}{\sqrt{2\pi}} e^{\frac{s^2}{4b}} \int_{-\infty}^{+\infty} a e^{-b\left(x+\frac{s}{2b}\right)^2} dx, \tag{2.37}$$

changing variables by $x(u) = u - \frac{s}{2b}$.
The determinant of the Jacobian of this transformation is 1. Thus,

$$B(s) = \frac{1}{\sqrt{2\pi}} e^{\frac{s^2}{4b}} \int_{-\infty}^{+\infty} a e^{-bu^2} du. \tag{2.38}$$

By using eqn.(2.16) the integral is solved as,

$$B(s) = \frac{1}{\sqrt{2\pi}} e^{\frac{s^2}{4b}} a \sqrt{\frac{\pi}{b}} \tag{2.39}$$

$$= \frac{a}{\sqrt{2b}} e^{\frac{s^2}{4b}}. \tag{2.40}$$

The associated Fourier transform is then:

$$F(w) = B(iw)$$

$$\frac{a}{\sqrt{2b}} e^{-\frac{w^2}{4b}}. \tag{2.41}$$

Thus, the Fourier transform of a Gaussian function is another Gaussian function.

2.2.4 Many-Gaussians Wave Packet

In quantum mechanics, a many-Gaussians wave packet is a wave packet that is constructed from a combination of multiple Gaussian wave packets. A Gaussian wave packet is a type of wave packet that is characterized by a Gaussian probability distribution function, and it is often used to model the behavior of particles in quantum systems because it is relatively simple and easy to work with mathematically. Many-Gaussians wave packets are often used to model the behavior of particles in complex quantum systems, such as molecules and solids. They can be used to study phenomena such as quantum coherence and quantum tunneling, and they are a useful tool for understanding the behavior of particles in various quantum systems as focused in this thesis.

Why Many-Gaussians Wave Packets are Useful?

Many-Gaussians wave packets are useful because they can capture more of the complexity of the system being modeled compared to single Gaussian wave packets. In general, many-Gaussians wave packets are more accurate than single Gaussian wave packets because they can represent the behavior of particles in complex quantum systems more accurately. For example, many-Gaussians wave packets can be used to model the behavior of particles in molecules and solids, which are more complex quantum systems than atoms or simple quantum wells. In addition, many-Gaussians wave packets can be used to study the behavior of particles in systems with multiple energy levels or multiple quantum states. This is because they can capture the

superposition of multiple quantum states, which is not possible with single Gaussian wave packets.

Mathematical Formalism

We develop many Gaussians wave function to solve our Open and Closed Quantum systems, defined as,

$$g(x) \equiv x_0 \sum_j e^{a_0(x-x_j)^2}, \tag{2.42}$$

where,

$$x_0 \equiv \frac{1}{(2\pi)^{1/4}\sqrt{a}}, \tag{2.43}$$

$$a_0 \equiv \frac{1}{4a^2} \tag{2.44}$$

a is the uncertainty in width such that $a \approx \triangle x$. Eqn.(2.18) gives Figure 2.1 and Figure 2.2

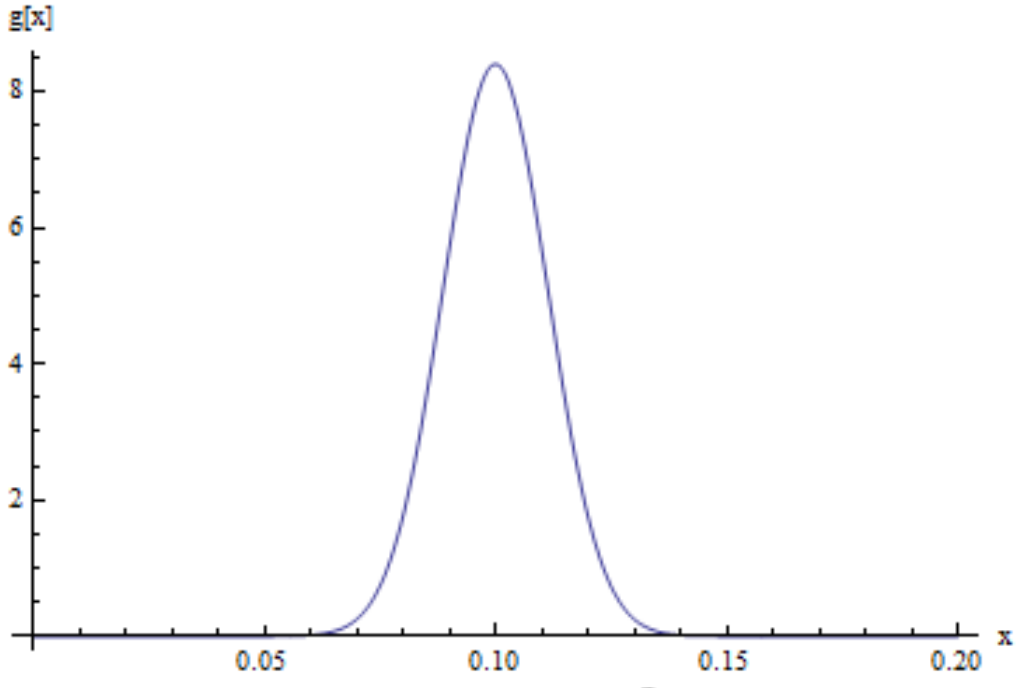

Figure 2.1: A Gaussian wavepacket centered at 0.10 For $a = 0.04L$.

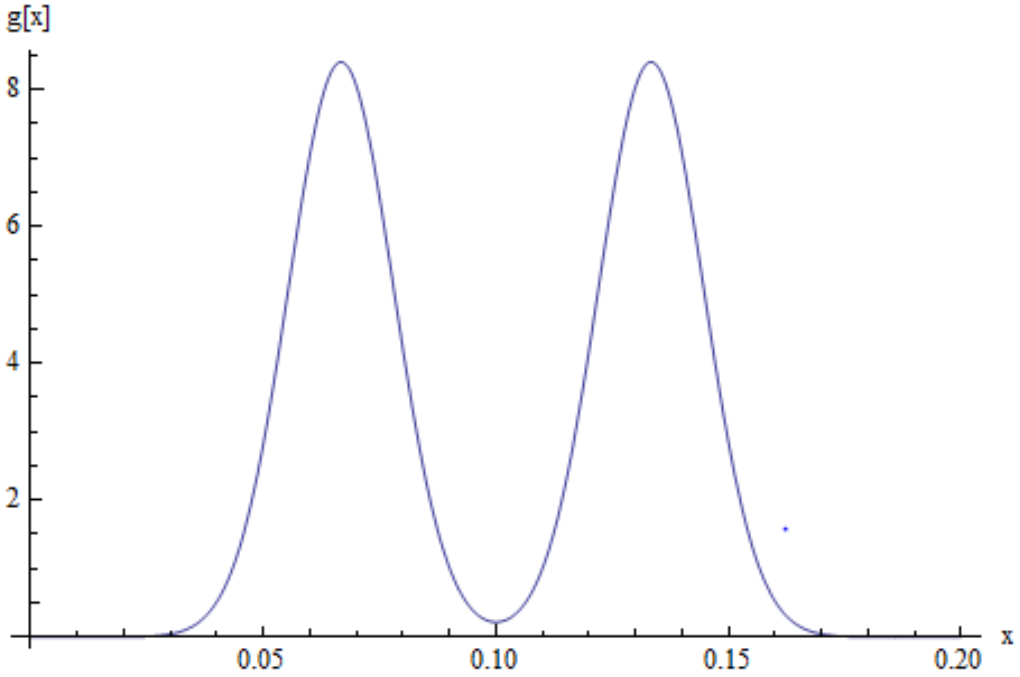

Figure 2.2: Two Gaussian wavepackets eqn.(2.18) whose peaks are 0.06m apart from each other For $a = 0.04L$.

From Figures (2.1) and (2.2) it is indicated that we can develop many Gaussian wavepakets for our desired Quantum systems.

2.3 Time Evolution of a Free Wave Packet

In this section we will accomplish a mathematical model for our Quantum Systems. Here, Our goal is to find the time evolved state $w(x,t)$ when we know the initial wavefunction $w(x,0)$ at $t = 0$.

Step 1. We will use $w(x,0)$ to compute $\mu(k)$.

$$\mu(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx w(x,0) e^{-ikx}, \tag{2.19}$$

Step 2. Using $\mu(k)$ to to rewrite $w(x,0)$ as a superposition of plane waves:

$$w(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \mu(k) e^{ikx}. \tag{2.20}$$

This is useful because we know how plane waves evolve in time. The above is called the Fourier representation of $w(x,0)$

Step 3. A plane wave $\mu_k(x,0) = e^{ikx}$ evolves in time into $\mu_k(x,t) = e^{i(kx-\omega(k))t}$ with $\hbar\omega = \frac{\hbar^2 k^2}{2m}$. Using superposition we see that eqn.(2.20) evolves into,

$$w(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \mu(k) e^{i(kx-\omega(k))t} dk \tag{2.21}$$

This is in fact the answer for $\mu(x,t)$. We can easily confirm that is the solution because; (i) it solves the Schrodinger equation and (ii) setting $t = 0$ in $\mu(x,t)$ gives us the initial wavefunction given by eqn.(2.20) that represented the initial condition.

Chapter 3

Model Systems

In this chapter we will construct a mathematical model that help us in understanding quantum systems. In this context we construct the free particle Schrodinger equation and then expand its formalism for particle in a potential. In this regard we use it for infinite square well.

3.1 Wave Function

In quantum mechanics, the wave function is a mathematical function that describes the probability amplitude of finding a particle at a particular location and time. It is a complex-valued function that is denoted by w in this thesis and is often referred to as the "quantum state" of the particle or system. The wave function is related to the wave packet through the Heisenberg uncertainty principle, which states that the more accurately we know the position of a particle, the less accurately we can know its momentum, and vice versa. This uncertainty is due to the wave-like nature of particles in quantum systems, and it is a fundamental aspect of quantum mechanics.

3.1.1 Equations for a Wave Function

The wave function or de Broglie wave for a particle with momentum p and energy E is given by,

$$w(x,t) = e^{i(kx-\omega t)} \tag{3.1}$$

where, ω and k are determined from,

$$p = \hbar k, E = \hbar\omega, E = \frac{p^2}{2m}. \tag{3.2}$$

The wavefunction in eqn.(3.1) represents a state of definite momentum. It is then of interest to find an operator that extracts that information from the wavefunction. We take,

$$\frac{\hbar}{i}\frac{\partial}{\partial x}w(x,t) = \frac{\hbar}{i}(ik)w(x,t) = pw(x,t) \tag{3.3}$$

where p is the momentum. Identifying the operator, $\frac{\hbar}{i}\frac{\partial}{\partial x}$ as the momentum operator $\hat{p}$,

$$\hat{p} \equiv \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{3.4}$$

$$\hat{p}w = pw \tag{3.5}$$

We can see that operating the $\hat{p}$ on the wavefunction $w(x,t)$ for a particle of momentum p, it gives p times the wavefunction. We say that w is an **eigenstate** of $\hat{p}$. Extracting the energy information from the free particle wavefunction,

$$i\hbar\frac{\partial}{\partial t}w(x,t) = i\hbar(-i\omega)w(x,t) = \hbar\omega w(x,t) = Ew(x,t). \tag{3.6}$$

Writing energy in terms of momentum for a free particle,

$$Ew = \frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}w$$

which suggests the following definition of the energy operator,

$$\hat{E} \equiv \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \tag{3.8}$$

This also allows us to find a differential equation for which our de Broglie wavefunction is a solution. Considering eqn.(3.6) and replacing the right

hand side Ew by $\hat{E}w$ gives us,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) \tag{3.9}$$

This is the **free-particle Schrodinger equation**. Interms of energy operator, it can be written as

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{E}\psi(x,t) \tag{3.10}$$

3.2 Schrodinger Equation for Particle in a Potential

If our quantum particle is moving in some external potential $V(x,t)$. In such case, the total energy of the particle is the sum of kinetic and potential energies,

$$E = \frac{p^2}{2m} + V(x,t) \tag{3.11}$$

Here, energy operator can be written as

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(x,t). \tag{3.12}$$

The Schrodinger equation for a particle in a potential takes the form,

$$i\hbar\frac{\partial}{\partial t}w(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)w(x,t) \tag{3.13}$$

The energy operator $\hat{E}$ is usually called the **Hamiltonian operator** $\hat{H}$,

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t) \tag{3.14}$$

and the Shrodinger equation becomes,

$$i\hbar\frac{\partial}{\partial t}w(x,t) = \hat{H}w(x,t) \tag{3.15}$$

From here we get a postulate of Quantum Mechanics that, "The time evolution of a quantum system is determined by the Hamiltonian or total energy operator $H(t)$ through the Schrodinger equation"
In **Dirac notation** eqn.(3.15) can be written as,

$$i\hbar\frac{d}{dt}|w(t)\rangle = H(t)|w(t)\rangle \tag{3.16}$$

The eigenvalues of the Hamiltonian are the allowed energies of the quantum system, and the eigenstates of H are the energy eigenstates of the system. Energy eigenvalue equation is,

$$H|E_n\rangle = E_n|E_n\rangle \tag{3.17}$$

The eigenvectors of the Hamiltonian form a complete basis because it is an observable, and therefore a Hermitian operator. Therefore, we consider the energy eigenstates as the basis of choice for expanding general state vectors,

$$|w(t)\rangle = \sum_n c_n(t)|E_n\rangle \tag{3.18}$$

which is orthonormal,

$$\langle E_k|E_n\rangle = \delta_{kn} \tag{3.19}$$

where, $c_n(t)$ is called expansion coefficients.
Substituting this general state into eqn.(3.16) we get,

$$i\hbar\frac{d}{dt}\sum_n c_n(t)|E_n\rangle = H\sum_n c_n(t)|E_n\rangle$$

using eqn.(3.17) we get,

$$i\hbar\sum_n \frac{dc_n(t)}{dt}|E_n\rangle = \sum_n c_n(t)E_n|E_n\rangle.$$

Using eqn.(3.19) and then collapses the sums we get,

$$\langle E_k|i\hbar\sum_n \frac{dc_n(t)}{dt}|E_n\rangle = \langle E_k|\sum_n c_n(t)E_n|E_n\rangle$$

$$i\hbar\frac{dc_k(t)}{dt} = c_k(t)E_k.$$

We get here a single differential equation, for each of the possible energy states of the systems $k = 1, 2, 3, \ldots$. This 1st-order differential equation can be rewritten as,

$$\frac{dc_k(t)}{dt} = -i\frac{E_k}{\hbar}c_k(t) \tag{3.20}$$

whose solution is a complex exponential given by,

$$c_k(t) = c_k(0)e^{-iE_kt/\hbar}. \tag{3.21}$$

The time-dependent solution for the full state vector can be obtained if the initial state of the system at time $t = 0$ is,

$$|w(0)\rangle = \sum_n c_n|E_n\rangle. \tag{3.22}$$

The time evolution of this state under the action of the time-independent Hamiltonian H is,

$$|w(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|E_n\rangle. \tag{3.23.A}$$

Translating the Dirac notation equations to wave function notation,

$$w(x,t) = \sum_n c_c\mu_n(x)e^{-iE_nt/\hbar}. \tag{3.23.B}$$

The c_n (i.e., the probability amplitudes), in wave function language are,

$$c_n = \int_{-\infty}^{+\infty} \mu_n(x)w(x,0)dx. \tag{3.23.C}$$

Eqn.**(3.23.A)**, eqn.**(3.23.B)** and eqn**(3.23.C)** will help us in solving open and closed Quantum systems in upcoming sections.

3.3 Particle Inside a Box

One of the simplest problems in quantum mechanics is a single free particle confined inside a one-dimensional box of length L. The potential energy is zero inside the box but infinite at the boundaries $x = 0$ and $x = L$. Schrodinger equation inside the box

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right) w = Ew \tag{3.24}$$

reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2w}{dx^2} = Ew. \tag{3.25}$$

The particle always remains inside the box because of the infinite potential barrier at the walls. So the probability of finding the particle outside the box is zero,i.e., $w = 0$ outside the box. The wavefunction is continuous at the boundaries of the potential well at $x = 0$ and $x = L$. This satisfies the boundary conditions

$$w(0) = w(L) = 0. \tag{3.26}$$

Eqn.(3.25) can be solved by using these boundary conditions as follows,

$$\frac{d^2w}{dx^2} + k^2w = 0$$

where,

$$k = \sqrt{\frac{2ME}{\hbar^2}}.$$

The general solution of this equation is given by,

$$w(x) = Asinkx + Bcoskx,$$

where A and B are constants that can be determined from the boundary conditions as well as normalization. The condition that $w(0) = 0$ leads to $B = 0$. Therefore,

$$w(x) = Asinkx.$$

The condition that $w(L) = 0$ gives,

$$Asin\,(kL) = 0.$$

This equation can be satisfied in two different ways. First is to choose $A = 0$. But this leads to $w(x) = 0$, which is not possible as it implies that particle is not inside the box. The other possibility is that

$$kL = n\pi,$$

where n=1,2,... are integers. Thus the solutions for the wavefunction are

$$w_n(x) \equiv \mu(x) = Asin\left(\frac{n\pi}{L}x\right). \tag{3.27}$$

The constant A can be found from the condition that the particle is somewhere inside the box,i.e.,

$$\int_0^L |w_n(x)|^2 dx = 1.$$

$$A^2 \int_0^L sin^2\left(\frac{n\pi}{L}x\right) = A^2\frac{L}{2} = 1$$

The normalization constant A is equal to $\sqrt{2/L}$. The normalized energy eigen states become,

$$\mu(x) = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi}{L}x\right) \tag{3.28}$$

By substituting the value of k, we get the energy of particle as follows

$$E_n = \frac{n^2\pi^2\hbar^2}{2ML^2}, \text{n=1,2,3, ...} \tag{3.29}$$

These allowed energies scale with the square of the quantum number n and produce the set of energy levels.

Chapter 4

Quantum Wave Packet Revivals and Quantum Dynamics in Open and Closed Quantum Systems

In this chapter we will track down the discussions about quantum revivals and classical periodicity. Here we will discuss the overlap of a time-dependent quantum mechanical wave function, $w(x,t)$, with its initial value, $w(x,0)$. Moreover, we will investigate the quantum dynamics of open and closed quantum systems in space and time.

4.1 Introduction

The study of quantum mechanics and its phenomena has been a central area of research in physics since its inception in the early 20th century. The revival of wave packets, which refers to the reformation of a quantum wave packet after it has spread out, was first studied by Schrödinger [3]-[6] in the 1920s. Schrödinger used the mathematical framework of quantum mechanics to describe the behavior of wave packets and showed that they could exhibit periodic revivals.

In the decades that followed, the revival of wave packets became a topic of

interest for many physicists, and numerous studies were conducted to better understand this behavior. In the 1970s and 1980s, several researchers studied the revival of wave packets in various physical systems, including the hydrogen atom and harmonic oscillators[7]-[10]. In recent years, the revival of wave packets has been the subject of renewed interest, due in part to advances in technology that have made it possible to experimentally observe these phenomena. With the development of ultra-cold atomic systems and optical lattices, it has become possible to study the revival of wave packets in well-controlled, highly tunable environments.

The use of the autocorrelation function as a tool to investigate the revival of wave packets is a relatively recent development, and its application to the study of one-dimensional boxes is a novel contribution to the field. This thesis builds on the existing body of knowledge and seeks to further our understanding of the revival of wave packets in a one-dimensional box by exploring the role of the autocorrelation function in this process.

The phenomenon of wave packet revivals, which has now been observed in many experimental situations, arises when a well-localized wave packet is produced and initially exhibits a short-term time evolution with almost classical periodicity (T_{cl}) and then spreads significantly after a number of orbits, entering a so-called collapsed phase where the probability is spread (not uniformly) around the classical trajectory. On a much longer time scale after the initial excitation, however, called the revival time (with $T_{rev} \gg T_{cl}$), the packet relocalizes, in the form of a quantum revival, in which the spreading reverses itself and the classical periodicity is once again apparent. Even more interestingly, many experiments have since observed additional temporal structures, with smaller periodicities (fractions of T_{cl}), found at times equal to rational fractions of the revival time (pT_{rev}/q). These have been elegantly interpreted [8] as the temporary formation of a number of 'mini-packets' or 'clones' of the original packet, often with $1/q$ of the total probability, exhibiting local periodicities T_{cl}/q, and have come to be known as fractional revivals. Observations of fractional revivals have been made in a number of atomic [11] - [16] and molecular [17] systems.

A simple picture [18] of the time-dependence of the quantum state leading to these behaviors, modeling the individual energy eigenstates and their

exponential $\left(e^{-iE_n t/\hbar}\right)$ time-dependent factors as an ensemble of runners or race-cars on a circular track, is often cited. The quantum mechanical spreading arises from the differences in speed, while the classical periodicity of the system is observable over a number of revolutions (or laps.) For longer times, however, the runners/race-cars spread out and no correlations (or clumpings) are obvious, while after the fastest participants have lapped their slower competitors (once or many times), obvious patterns can return, including smaller 'packs' of racers, clumped together, which model fractional revivals.

4.2 Collapse and Revival

In a one dimensional box that contains an initial wave packet as a Gaussian, when it is evolved in time, it first disperses, which we call the **Collapse** and then comes back to it's initial state in a specific amount amount of time, for which we coin the word **Revival**.

A classical Metaphor: Consider shuffling of an initially highly ordered deck of playing cards. One shuffling method involves splitting the deck into two equal halves, and then alternately placing the bottom card from each half into a pile, reforming and reordering the deck. After only a few such shuffles, the original order is seemingly completely lost and the cards appear to have randomized(this is like a collapse of state). After only a few more turns, however, clear patterns of ordered subsets of suits and ranks appear, increasingly so until after only eight such shuffles the deck has returned to its original highly ordered state(that resembles with revivals meaning revives).

Why Revivals Occur? The very simple answer is "**Degeneracy**."
"Every Closed Quantum System is degenerate". Greater the degeneracy is, richer the space-time dynamics are.

4.2.1 Quantum Revivals and Classical Periodicity

The classical limit of quantal time development, first studied by Ehrenfest is still an area of active investigation. Much of this research centers on

systems with two or more degrees of freedom, where classical chaos enters the picture, and much centers on approximate quantal revivals in complicated situations. Yet this section will show that even that workhorse of introductory quantum mechanics, namely the one-dimensional infinite square well(Discussed in previous chapter), exhibits surprising features, the elucidation of which contributes to one's intuition concerning quantum mechanics and illuminates the more general problems. The topic of quantal time development in the infinite square well has been treated theoretically by Bluhm, Kostelecky and Porter by Aronstein and Stroud[19-21]. In these treatments the results flow ultimately either from the WKB approximation or from a sophisticated Taylor series expansion of the eigenenergies E_n as a function of the integer quantum number n. A particle of mass M moves in an infinite square well of width L, centered on the origin. This system has energy eigenvalues given by,

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2ML^2} \tag{4.1}$$

As the energy increases, the separation between energy eigenvalues increases rather than decreasing to a continuum as is usual, and as is expected for the classical limit. It is a trivial matter to show that a classical particle of energy E in the infinite square well bounces back and forth between the walls with period

$$T_{cl} = L\sqrt{\frac{2M}{E}} \tag{4.2}$$

Suppose the initial wave function is,

$$w(x,0) = \sum_n c_n \mu_n(x)$$

Some of the expansion coefficients c_n may of course vanish. This wave function evolves in time to,

$$w(x,t) = \sum_n c_n \mu_n(x) e^{-iE_n t/\hbar}$$

Does it ever happen that at some revival time T_{rev} the quantum state represented by $w(x,t)$ is exactly the same as the initial state $w(x,0)$?

Such a revival will happen whenever all of the phase factors $e^{-iE_n t/\hbar}$ are equal. Noting that the phase factors do not all have to equal one, because the two wave functions $w(x)$ and $e^{-i\mu}w(x)$ represent the same quantum state. That is, it happens whenever,

$$\frac{E_n}{\hbar}T_{rev} = 2\pi N_n + \mu \tag{4.3}$$

for all n such that $c_n \neq 0$.
Here, N_n is an integer, positive, negative, or zero, that can vary from one value of n to another, whereas the time T_{rev} and the phase μ is not varying with n. Using the eigen energy result $E_n = E_1 n^2$, gives

$$T_{rev} = \frac{\hbar}{E_1}\left[2\pi\frac{N_n}{n^2} + \frac{\mu}{n^2}\right] \tag{4.4}$$

We will have found a revival if we can make the right-hand side independent of n. As, $\frac{\mu}{n^2}$ will be independent of n only when either $(1)\mu = 0$ or
else (2) only special values of n enter the superposition. The ratio $\frac{\mu}{n^2}$ can be made independent of n by selecting,

$$N_n = (\text{integer})n^2 \tag{4.5}$$

and the smallest such integer is one.
We have proven,

Theorem 1: Exact Quantum Revivals

Any wave function in an infinite square well will exactly come back to itself after a time,

$$T_{rev} = \frac{2\pi\hbar}{E_1} = \frac{4ML^2}{\pi\hbar} \tag{4.6}$$

Theorem 2: Reflection Half-Way to a Revival

After the passage of half a revival time, any wave function is reflected about the origin (with a physically irrelevant change of sign),

$$w(x, T_{rev/2}) = -w(-x, 0) \tag{4.7}$$

Theorem 3: Mock Rabi Oscillations

If the wave function is a superposition of only two energy eigenfunctions, namely n and m, then it revives after the shorter time,

$$\tau_{n,m} = \frac{T_{rev}}{m^2 - n^2} = \frac{2\pi\hbar}{E_m - E_n} \tag{4.8}$$

at which time,

$$w(x, \tau_{n,m}) = e^{-2\pi i n^2/(m^2-n^2)} w(x, 0) \tag{4.9}$$

$$w(x, \tau_{n,m}) = e^{-2\pi i m^2/(m^2-n^2)} w(x, 0) \tag{4.10}$$

Note the physically irrelevant change of phase.

Theorem 4: If a wave function has odd parity, it revives after the passage of time $T_{rev}/4$,

$$w_0(x,)T_{rev}/4 = w_0(x, 0) \tag{4.11}$$

Theorem 5: If a wave function has even parity, it revives after the passage of time $T_{rev}/8$

$$w_e(x,)T_{rev}/8 = e^{-i\pi/4} w_e(x, 0) \tag{4.12}$$

Theorem 6: If a wave function is a superposition of a finite number of energy eigenstates, namely n_a,n_b,n_c,n_d,...,n_z, then its first revival comes at time,

$$\tau = \frac{T_{rev}}{GCD\left[n_b^2 - n_a^2, n_c^2 - n_a^2, n_d^2 - n_a^2, ..., n_z^2 - n_a^2\right]} \tag{4.13}$$

where "GCD" signifies the greatest common divisor.

Theorem 7: The wave function is a superposition of energy eigenstates with energies (listed from smallest to largest)

E_a, E_b, E_c,E_d,...,E_z. Then the quantum state will recur exactly at a time τ when the phase factors $e^{-iE_a\tau/\hbar}$,$e^{-iE_b\tau/\hbar}$,$e^{-iE_c\tau/\hbar}$, $e^{-iE_d\tau/\hbar}$,...,$e^{-iE_z\tau/\hbar}$ are all equal.

4.3 Autocorrelation Functions(ACF)

The autocorrelation function is a mathematical tool used to describe the temporal behavior of a quantum system. It is a measure of the similarity between a quantum state at two different times and is defined as the inner product of the state at the initial time with the state at a later time. The autocorrelation function can be used to study the dynamics of a quantum system and to determine if it is in a stable or unstable state. It can also be used to detect quantum interference effects and to analyze the coherence properties of a quantum system.

4.3.1 Mathematical Interpretation

The autocorrelation function in quantum mechanics is mathematically represented as the inner product of the wave function of a quantum system at time t_1 with the complex conjugate of the wave function at a later time t_2. The wave function, denoted as $w(t_1)$ and $w(t_2)$, describe the state of a quantum system and contains information about the position and momentum of the particles in the system. The autocorrelation function is given by,

$$C(t_1, t_2) = \langle w(t_1)|w(t_2)\rangle \tag{4.14}$$

where $\langle w(t_1)|$ is the bra vector of the wave function at time t_1 and $|w(t_2)\rangle$ is the ket vector of the wave function at time t_2. The inner product $\langle w(t_1)|w(t_2)\rangle$ gives the probability amplitude for the system to be in the state $w(t_1)$ at time t_1 and in the state $w(t_2)$ at time t_2.
The autocorrelation function can be used to study the temporal behavior of a quantum system, the dynamics of the system and detect the coherence

property of the system. Also, it can be used to study the interference effects on the system.

4.3.2 Density matrix Formulasim

The density matrix formulation of the autocorrelation function is given by the expectation value of the product of the initial density matrix, $\rho(0)$, and the density matrix at a later time, $\rho(t)$, in the following,

$$C(t) = Tr[\rho(0)\rho(t)] \tag{4.15}$$

Where Tr denotes the trace operation and $C(t)$ is the autocorrelation function at time t. This formulation allows one to calculate the autocorrelation function for a mixed state, which is a statistical ensemble of pure states. The density matrix formulation is also useful for studying systems with a large number of degrees of freedom and for understanding the decoherence and relaxation processes in quantum systems.

4.3.3 Autocorrelation Function and Quantum Revivals

Autocorrelation functions and quantum revivals are related in the sense that both deal with the time evolution of quantum systems. Quantum revivals refer to the phenomenon where a quantum system returns to its initial state after a certain period of time. This can occur when the system is described by a wave function that is periodic in time, such as a wave function that is a superposition of a discrete set of energy eigenstates. In the case of a system experiencing quantum revivals, the autocorrelation function will show maxima at the times when the system is returning to its initial state. The maxima of the autocorrelation function correspond to the times when the system is most similar to its initial state. In other words, the autocorrelation function can be used to detect and quantify the phenomenon of quantum revivals by measuring how similar the system is to its initial state at different times. It's worth mentioning that, for a system that does not show revivals, the autocorrelation function will generally decay exponentially over time, indicating that the system becomes increasingly dissimilar from its

initial state. The autocorrelation function, on the other hand, is a measure of the similarity between the initial state of a system and its state at a later time. The mathematical relation between the autocorrelation function and quantum revivals can be described as follows: The autocorrelation function is defined as,

$$C(t) = \langle w(0)|w(t)\rangle \tag{4.16}$$

Where $w(0)$ is the initial state of the system and $w(t)$ is the state of the system at time t. For a system experiencing quantum revivals, the wave function $w(t)$ can be written as a superposition of energy eigenstates,

$$w(x,t) = \sum_n \mu_n(x) c_n e^{-iE_n t/\hbar} \tag{4.17}$$

Where c_n are the coefficients of the wave function and E_n are the energy eigenvalues. Substituting this into the autocorrelation function, we get,

$$C(t) = \sum_n |c_n|^2 e^{-iE_n t/\hbar} \tag{4.18}$$

This shows that the autocorrelation function will have maxima at times when the system is returning to its initial state. In other words, when the system is in its initial state, the autocorrelation function is 1. When the system is not in the initial state, the autocorrelation function will be less than 1 and will show maxima when the system is returning to the initial state, this maxima is known as quantum revivals. It's worth mentioning that this is an idealized case and in practice, the system may not show perfect revivals due to various reasons such as decoherence, noise, etc. The auto correlation function can be written by using Taylor's expansion of energy E_n around n_0. This leads us to calculate the times T_0^j, at which the system exhibits recurrences. Times can be written as,

$$T_0^{(j)} = \frac{2\pi\hbar}{\frac{1}{j!}|E_n^{(j)}|}$$

Where,

$$E_n^{(j)} \equiv \frac{\partial^j E_n}{\partial n^j}|_{n=n_0}$$

It describes the jth derivative of the energy with respect to the principal quantum number n.
For $j = 1$;

$$T_0^{(1)} = 2\pi\hbar \left(\frac{\partial E_n}{\partial n} \right)^{-1}$$

This corresponds to the classical period of the wave packet.
In terms of classical action $I = n\hbar$

$$T_0^{(1)} = 2\pi \left(\frac{\partial E_I}{\partial I} \right)^{-1}$$

For $j = 2$;

$$T_0^{(1)} = 2\pi\hbar \left(\frac{1}{2} \frac{\partial^2 E_n}{\partial n^2} \right)^{-1}$$

This yields the quantum mechanical revival time of the wave packet in potential. In terms of classical action $I = n\hbar$

$$T_0^{(1)} = 2\pi \left(\frac{\hbar}{2!} \frac{\partial^2 E_I}{\partial I^2} \right)^{-1}.$$

The plot shown in Figure 4.1 will start at 1 when $t = 0$, as the autocorrelation function measures the similarity between the initial state and the state at time t, and when $t = 0$, the system is in its initial state. As the time increases, the autocorrelation function will decrease, indicating that the system is becoming less similar to its initial state. At certain specific times, known as the revival times, the autocorrelation function will show maxima, indicating that the system is returning to its initial state. Between the revival times, the autocorrelation function will decrease exponentially, indicating that the system is becoming increasingly dissimilar from its initial state. The amplitude of the maxima will be less than 1, indicating that the system is not returning to its initial state perfectly. As time increases, the frequency of the maxima will decrease, indicating that the system is not returning to its initial state as frequently.

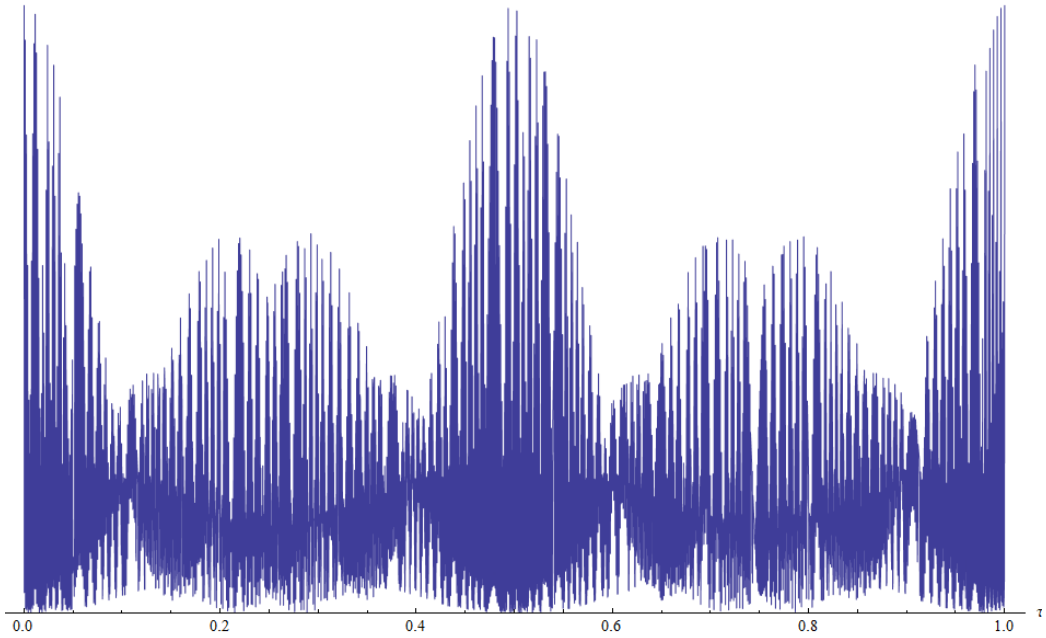

Figure 4.1: Plot of the autocorrelation function, $|C|^2$.

4.3.4 ACF for Gaussian Distribution

If the coefficients c_n of the wave function are described by a Gaussian distribution in terms of the quantum number n, the autocorrelation function can be written as:

$$C(t) = \sum_n \frac{1}{\sqrt{2\pi}\triangle n} e^{-\frac{(n-n_0)^2}{2\triangle n^2}} e^{-iE_n t/\hbar} \tag{4.19}$$

where, we have introduced c_n as a Gaussian distribution in n as

$$c_n = \frac{1}{\sqrt{\triangle n\sqrt{2\pi}}} e^{-\frac{(n-n_0)^2}{4\triangle n^2}}$$

Which gives the required normalization,

$$\sum_0^\infty |c_n|^2 \approx 1.$$

If the coefficients c_n of the wave function are described by a Gaussian distribution in terms of the quantum number n, the plot shown in Figures 4.2 and 4.3 of the autocorrelation function will have similar characteristics to the idealized case.

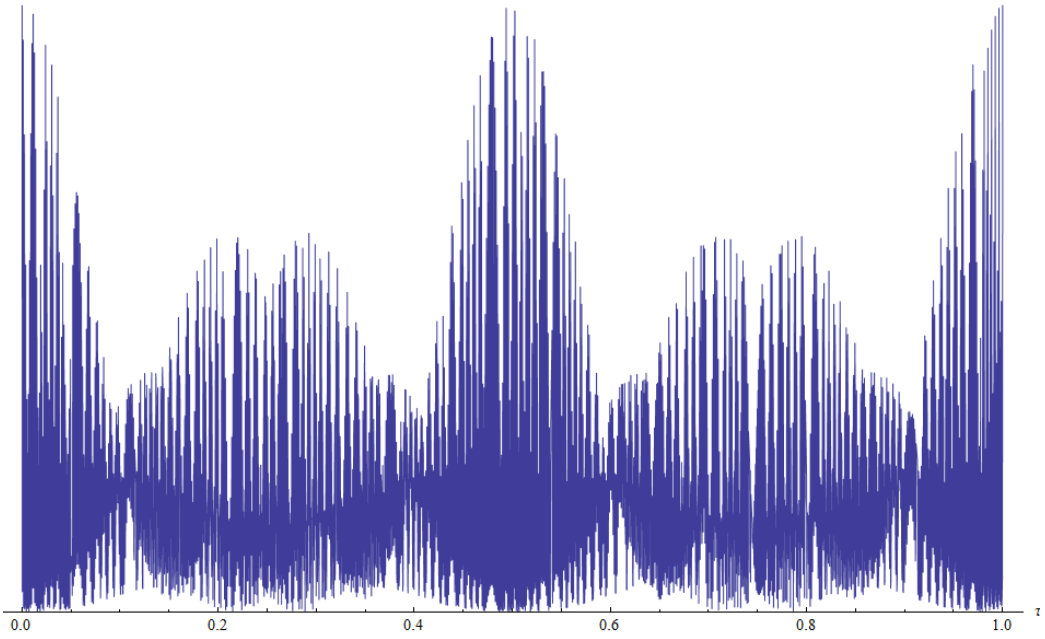

Figure 4.2: Characteristic time dependences of the auto-correlation function of the wave packet for quantum number 1 to 15. Here we have used c_n as Gaussian distribution in n.

4.4 Quantum Dynamics in Open and Closed Quantum Systems

In this section I will discuss the space-time dynamics(STD) in open and closed quantum systems. We will investigate the spacatio-temporal behaviour of quantum mechanical probability density.

4.4.1 Space-Time Dynamics in Closed Quantum Systems

Here I will track down the formation of Quantum interference patterns, that can be seen as the regular patterns due to the evolution of quantum mechanical probability in space and time. Eqn.(3.28) gives the normalized energy eigen states as,

$$\mu_n(x) = k_0 \left[\frac{e^{ik_n x} - e^{-ik_n x}}{2i} \right] \tag{4.20}$$

We introduced,

$$k_n \equiv \frac{n\pi}{L} \tag{4.21}$$

k_n represents the wave number. And

$$k_0 \equiv \sqrt{\frac{2}{L}}. \tag{4.22}$$

In wave function language from eqn.(3.23C) we get,

$$c_n = \int_0^L \mu_n(x) g(x) dx. \tag{4.23}$$

The initial wave packet vanishes at the walls at $x = 0$ and $x = L$. Moreover, it vanishes outside of the box. We can therefore extend the integral in definition of the expansion co-efficients to $-\infty$ and $+\infty$, that is

$$c_n = \int_{-\infty}^{+\infty} \mu_n(x) g(x) dx. \tag{4.24}$$

By inserting the values and solving the integral we get,

$$c_n = c_0 e^{\frac{-k_n^2}{4a_0}} \times \sum_j sin\,(k_n x_j) \tag{4.25}$$

I've defined,

$$c_0 \equiv x_0 k_0 \times \sqrt{\frac{\pi}{a_0}}. \tag{4.26}$$

Quantum mechanical probability density after simplification can be written as,

$$P \equiv |w(x,t)|^2 = \Omega_0^2 \times \sum_n \sum_m \sum_j \sum_k \times e^{-\frac{k_n}{4a_0}} \times e^{\frac{-k_m}{4a_0}}$$
$$sin\,(k_m x_k) \times sin\,(k_n x_j) \times sin\,(k_m x) \times sin\,(k_n x)$$
$$e^{-iE_n t\hbar} \times e^{+iE_m t\hbar}$$

where,

$$\Omega_0^2 \equiv \frac{4\pi\sqrt{2}}{aL^2}. \tag{4.27}$$

Energy In Terms of Quantum Revival

$$E_n = \frac{(\hbar k_n)^2}{2M} = n^2 E_1 = n^2 \hbar\omega_1$$

$$E_n = n^2 \hbar \frac{2\pi}{T}$$

from Theorem-1 eqn.(4.6) we have

$$T \equiv \frac{4ML^2}{\pi\hbar}$$

which represents the revival time, in which the wave function is identical to its initial form at $t = 0$ so that,

$$w(x, t = T) = w(x, t = 0).$$

Simplifying

$$e^{-\frac{it}{\hbar}(E_n - E_m)} = e^{-\frac{it}{\hbar}(n^2\hbar\frac{2\pi}{T} - m^2\hbar\frac{2\pi}{T})}$$
$$e^{-\frac{it}{\hbar}(E_n - E_m)} = e^{-i2\pi(n^2 - m^2)\frac{t}{T}}.$$

Also,

$$e^{-\frac{1}{4a_0}(k_n^2 + k_m^2)} = e^{-(\frac{a\pi}{L})^2\left[n^2 + m^2\right]}.$$

Interestingly, it can de distinctly seen that the given equation of quantum mechanical probability involves the addition and subtraction of different powers

of quantum numbers as the argument of exponential functions. The summation over many quantum numbers, many of these arguments provide the identical constant, which results in **Quantum interference patterns** which can also be called Quantum Carpets. Which means larger the degeneracy is, richer the interference patterns are i-e., more arguments of exponential functions giving the same results.

To understand the quantum mechanical probability density we use density plot. Through out, the results are generated by introducing scaled coordinates for density plots as continuous function of space and time shown in Figure 4.4. For this purpose along x-axis we choose τ, defined as,

$$\tau \equiv \frac{t}{T},$$

while along y-axis we select ξ equivalent as,

$$\xi \equiv \frac{x}{L}.$$

We get the space time patterns, may also be called quantum carpets. Where, the diagonal lines are due to the interference between the terms in summations of final equation.

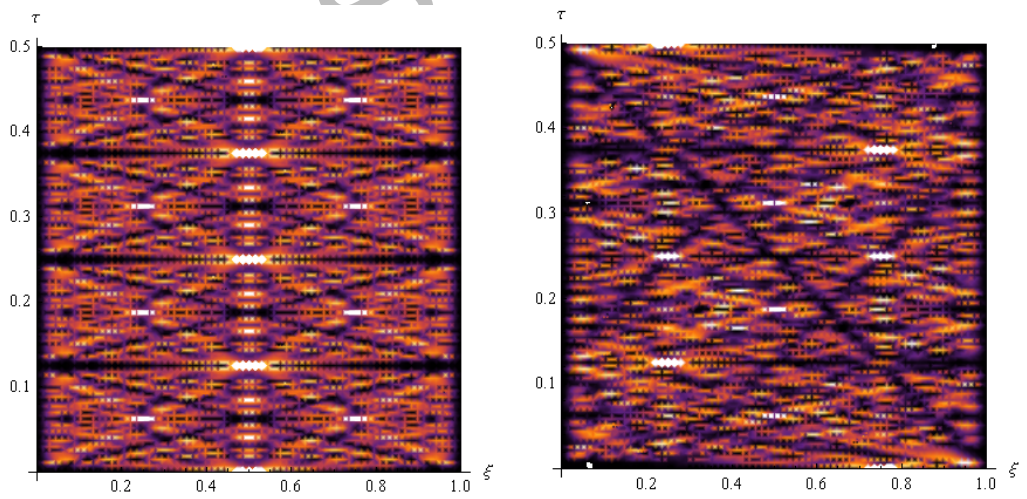

Figure 4.3: Density plot with initial width of Gaussian wave packet($a = 0.01L$) placed at $\frac{L}{2}$ [Left] and $\frac{3}{4}L$ [Right].

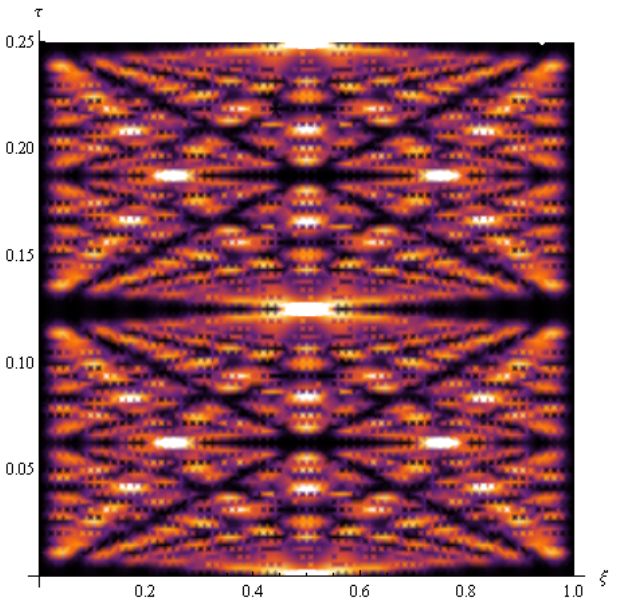

Figure 4.4: Density plot with initial width of Gaussian wave packet($a = 0.01L$) placed at $L/2$.

4.4.2 Space-Time Dynamics in Open Quantum System

Here, I will discuss the quantum mechanical probability for open quantum system in space and time. We will see the space time structures which appear due to the summation over number of Gaussians followlwed by the arguments of exponential i-e., x_j and x_k. For open quantum system I have considered many Gaussian wave packets. Here I will evolve these many Gaussian wave packets in time and will see the space-time behavior which weaves quantum structures. I have used x_j and x_k as the arguments of exponential functions for the case of many Gaussians wave function. For this purpose I will expand many Gaussians wave function in terms of energy eigen functions and then will reconstruct the wave function at a later time t by superposing the parts with appropriate phase factors.

$$w(x,t) = \int_{\infty}^{+\infty} \frac{dk}{\sqrt{2\pi}} \left[\mu(k) e^{ikx} e^{-iE_k t/\hbar}\right]. \tag{4.28}$$

After calculations we get the result,

$$w(x,t) = c_j \times \sum_j e^{-\frac{(x-x_j)^2}{4\triangle x^2(1+\eta^2t^2)}} \times e^{i\Omega(x,j)t} \tag{4.29}$$

here I have introduced,

$$\Omega(x,j) \equiv \frac{(x-x_j)\eta}{4\triangle x^2(1+\eta^2t^2)} \tag{4.30}$$

Ω has the dimensions of frequency and is a function of x and t. I call this "**The Space-Time parameter**". And

$$c_j \equiv \left(\frac{2a}{\pi}\right)^{1/4} \times \frac{1}{\sqrt{1+i\eta t}}. \tag{4.31}$$

Also,

$$\eta \equiv \frac{2\hbar a}{M}, \tag{4.32}$$

η has dimensions of T^{-1}, inverse of time. In density plots this parameter may be linked to Talbot distance where, $Z_T \equiv \frac{2\triangle x^2}{\lambda_{dB}}$, as distance at which the space-time images will be regularly repeated.
Finally the quantum mechanical probability density results,

$$P \equiv |w(x,t)|^2 = |c_j|^2 \times \sum_j \times \sum_k e^{-\frac{(x-x_j)^2}{4\triangle x^2(1+\eta^2t^2)} \times} e^{-\frac{(x-x_k)^2}{4\triangle x^2(1+\eta^2t^2)}} e^{i\Omega(x,j)t} \times e^{-i\Omega(x,k)t}. \tag{4.33}$$

Which explains the space-time dynamics in open quantum system. We can see that the space-time parameter plays a vital role in the formation of space-time images depicted in Figure 4.5. We examine the behavior of quantum mechanical probability density as given in eqn.(4.33), representing the dynamics of open quantum system in space and time. For this purpose we use density plots and introduce the scaled parameters as follows,

$$\xi \equiv \frac{x}{L}$$

along x-axis. While,

$$\tau \equiv \frac{t}{T}$$

along y-axis. Where, T is related to η, as introduced in eqn.(4.19), which may be linked to Talbot distance where, $Z_T \equiv \frac{2\triangle x^2}{\lambda_{dB}}$, is distance at which the space-time images will be regularly repeated.

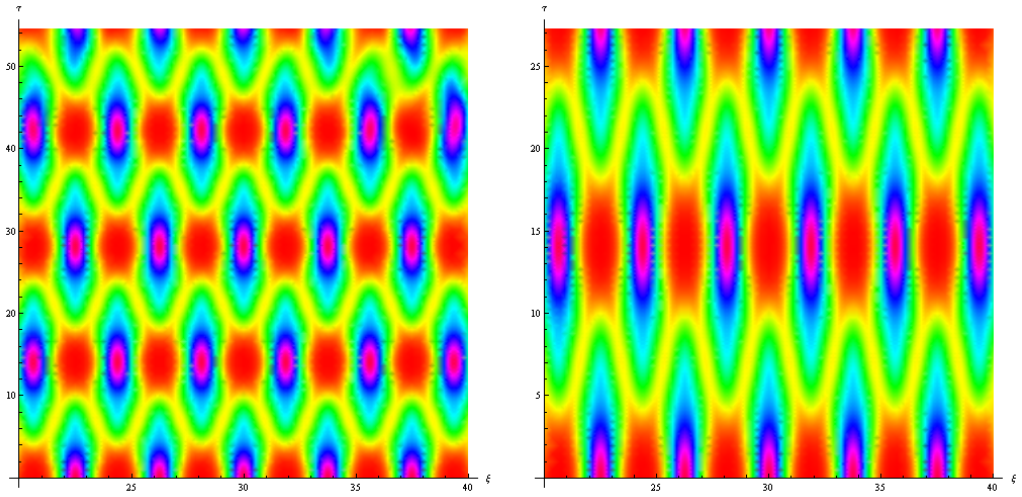

Figure 4.5: Density plot with initial width of Gaussian wave packet($a = 0.04L$) placed at $L/2$.

Chapter 5

Conclusion

In this thesis we have thoroughly explored the concept of quantum revivals in a one-dimensional box using the autocorrelation function. Our study has provided a detailed analysis of the temporal evolution of wave packets in a one-dimensional box and the occurrence of quantum revivals. The results of this research have expanded our understanding of the behavior of quantum systems and have important implications for a variety of fields, including quantum computing and quantum communication. The use of the autocorrelation function as a tool to study quantum revivals has proven to be highly effective, providing valuable insight into the fundamental principles of quantum mechanics. Our findings have demonstrated that quantum revivals are a robust and recurring phenomenon, and have provided a deeper understanding of the temporal behavior of wave packets in quantum systems.
Moreover, in this thesis we set up mathematical models for open and closed quantum systems. We build a many Gaussians wave packet and observed their space-time evolution in both quantum systems. In case of closed quantum system, we observe the formation of highly regular spatio-temporal or multidimensional patterns in the quantum mechanical probability $|w|^2$. This is due to pair interference between individual eigen-modes of the system forming the so called intermode traces. Moreover, from the expression of quantum mechanical probability, we can see that it involves the addition and subtraction of different powers of quantum numbers as the argument of exponential functions. The summation over many quantum numbers, many

of these arguments provide the identical constant, which result in quantum interference patterns. Which means larger the degeneracy is, richer the interference patterns are i-e., more arguments giving the same results.
In case of open quantum system, we observe space-time images. These are due to a key parameter to what I named space-time parameter $\Omega(x, j)$. If we throw a gleam of light on the expression of quantum mechanical probability, we see that different values of j and k contribute to interference patterns. In this case we relate the periodic distance with Talbot length.
Conclusively, we see that the formation of quantum interference patterns in closed quantum system is contributed due to summation over quantum numbers n, m and number of slits. But in comparison with open quantum system we distinctly marked that here the interference patterns are due to summation over many Gaussian wave functions each coming from different slits, acting like n, m. This is how an open quantum system differs from a closed quantum system.
On the basis of this we propose a model that may be helpful in experimental high energy physics for various experiments like a diffraction experiment in such a way that a grating can be built whose slits width would be controllable from our proposed model. In addition we may use any of particles whose interference patterns would lead us to the detailed information about a grating through which it has passed along.

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