Spatio-Temporal Dynamics of Wave Packet in Position-Dependent Effective Mass Systems

by

Sunia Javed

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Supervised by

Dr. Shahid Iqbal

School of Natural Sciences

National University of Sciences and Technology

Islamabad, Pakistan

FORM TH-4

National University of Sciences & Technology

MS THESIS WORK

We hereby recommend that the dissertation prepared under our supervision by: Sunia Javed, Regn No. NUST201463629MSNS78114F Titled: Spatio-temporal Wave Packet Dynamics in Position Dependent Effective Mass Systems be accepted in partial fulfillment of the requirements for the award of **MS** degree.

Examination Committee Members

1. Name: Dr. Aeysha Khalique Signature: Aeysha Khaliqueel.
2. Name: Dr. Muddasir Ali Shah Signature:
3. Name: Signature:
4. Name: Dr. Muhammad Ayub Signature:

Supervisor's Name: Dr. Shahid Iqbal Signature:

Aeysha Khaliqueel.
Head of Department

25-08-16
Date

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Date: 25/8/16

Dean/Principal

Dedication

It is dedicated to my father who has always been a great beacon of light and a source of endless inspiration for me; to my dear mother, whose encouragement and supportive hands has always added to my confidence to meet the challenges ahead.

Acknowledgement

In the name of Allah (S.W.T), the most Merciful, the most Gracious. I am thankful to the Lord of the whole universe, Allah (S.W.T), who supplied me with the courage to complete this research. Also, I cannot forget the most respectable personality for whom Allah (S.W.T) created the whole universe, Prophet Hazrat Muhammad (P.B.U.H).

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I wish to use this knowledge for the betterment of mankind. I pray for myself to be able to forward what I have learnt here.

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Abstract

Wave packet quantum dynamics in bounded one-dimensional systems manifests a lot of phenomena which have no analogue in classical dynamics, such as, the phenomena of quantum revivals and fractional revivals. In this thesis we explore these phenomena in the context of position-dependent effective mass systems (PDEM). Such systems have great importance in many areas of physics and have attracted a lot of attention most recently due to the possibility of fabricating them in laboratory. Nonetheless, the work presented in this thesis is focused on the theoretical investigations of wave packet revivals and fractional revivals in PDEM systems.

The quantization of position dependent effective mass systems and finding their solutions experience some mathematical and conceptual difficulties. In the first part we review various techniques of quantization and finding their solutions. We then apply the general formalism to find the solutions of a particle with position-dependent effective mass trapped in infinitely deep potential well. The Gaussian wave packet is then constructed by linear super-position of eigenfunctions of the PDEM system and its time evolution is studied.

The study of wave packet dynamics is of great interest due to occurrence of quantum revivals. An initially well localized wave packet follows the classical periodicity during short term time evolution. But after completing many classical periods phase difference among constituent waves lead to destructive interference which results in collapse when the phase difference is maximum. After that constructive interference takes place which becomes the cause of occurrence of quantum revivals.

We explore the wave packet dynamics by means of autocorrelation and temporal evolution of probability density of spatial wave packet−spatio-temporal dynamics. The image plots of temporal evolution of position-space probability density, known as quantum carpets, are presented to explore the structure of quantum revivals and fractional revivals. It is found that structure of fractional revivals is modified due to the spatially varying mass. In order to understand the effects of spatial-dependence on wave packet evolution, we have compared the results with corresponding constant mass systems. This leads us to conclude that spatial-dependence of mass modifies the design of quantum carpets and hence the structure of fractional revivals.

Contents

Chapter 1

Introduction

The quantum world shows very fascinating phenomenon which do not have corresponding analogue in classical world. Therefore the unambiguous distinction between these two theories is one of the philosophical question from the beginning of quantum theory. In this context, Erwin Schrödinger formulated wave mechanics as a possible analogue to classical mechanics. In this formalism, the dynamical state of a system is expressed by a mathematical function, known as wave function and the physical information about dynamical variables can be obtained from this function by specific operators. Moreover, he tried to build one-to one correspondence between classical-quantum dynamics of a system. He could succeeded to do so only for the harmonic oscillator and failed to generalized the notion. However, later it has been pointed out that there are several phenomena in quantum dynamics which do not have corresponding description in classical mechanics, known as non-classical phenomena.

In this thesis, we study the dynamics of a class of quantum mechanical systems whose mass is varying with position, named as, position-dependent effective mass systems (PDEM) and explore the non-classical phenomena namely, quantum revivals and fractional revivals. In the following we present a brief introduction about the main content covered in this thesis.

1.1 Position dependent effective mass systems

The concept of position dependent effective mass comes from many body systems in condensed matter physics [1–3]. Firstly, effective mass is needed to be understand. An electron in a crystal may behaves as if it has a mass different from the free electron mass m_0. This altered mass is known as effective mass. There exists some crystals in which the effective mass of the charge carrier is much larger or smaller than m_0. The effective mass may be anisotropic (which has different values when measured in different directions). The effective mass approach is also observed in the study of electronic properties of semiconductor [1, 2], quantum liquids, compositionally graded crystals [4], quantum dots [5–7], semiconductor heterostructures [8–14]. Due to advent in growing ultra thin semiconductor structure, position dependent effective mass theory has attracted attention.

Heterostructures are the building blocks of many semiconductor devices. The edge of heterostructures is that we can precisely control over the states and motion of charge carriers in semiconductors. A heterostructure is defined as a semiconductor structure in which the chemical composition changes with position. The simplest heterostructure has a single heterojunction, which is an interface within a semiconductor crystal across which the chemical composition changes. Most devices and experimental samples contain more than one heterojunctions as well.

Electron in a crystal (such as in semiconductors) is not completely free, but interacts with the potential of the lattice as this electron is in influence of other atoms present in the crystal as well. The quantum dynamics of such electrons can be modeled by considering position dependent effective mass system.

Classically, to write the Hamiltonian for position dependent effective mass systems, kinetic energy term involves both variables that are position and momentum in contrast to constant mass systems. An important point in this frame work is quantization of the spatially dependent mass systems. Main question is the transition of kinetic energy term $T(x, p)$ to the quantum one $\hat{T}(\hat{x}, \hat{p})$. This is done just by replacing the position and momentum observables by their corresponding quantum operators. Now, kinetic energy term in Hamiltonian involves both position and momentum operators, that do not commute with each other. Due to incom-

patible nature of position and momentum operators, kinetic energy term faces the ambiguity in ordering of $m(\hat{x})$ and $\hat{p}$.

To solve the ordering ambiguity, different ordering schemes are present in literature, that generate Hermitian Hamiltonians, such as Weyl ordering [15, 16], von Ross ordering [17, 18], Ki and Kuhn ordering [19] and Zhu and Kroemer ordering [20]. These ordering schemes give rise to non equivalent Hermitian Hamiltonians which are same at classical level. The most general one is the von Ross [17, 18] ordering in which position and momentum operators follow the constraint parameter. Several choices for these parameters are available but the most commonly used is given by Levy-Leblond [21]. This issue of ordering has been inscribed by several authors [22–26]. More specifically it has been discussed in the illustration of impurities in crystals [27, 28]. Finding solutions of any quantum mechanical system is an important task for the physical understanding of that system. One of the well known method is solving Schrödinger equation of that system. Some other methods are present in literature for finding the exact solutions of quantum system, such as shape invariance [29], potential algebras [30, 31], method of point canonical transformation [32, 33] and the path integral approach [34]. These all above mention methods have been used to solve constant mass system and as well as position dependent effective mass systems.

1.2 Solution of Schrödinger equation with PDM

Much attention has recently been paid to obtain exact solutions to quantum mechanical systems with PDEM due to the fact that they are useful in physical applications. Different methods have been used for quantum system with constant mass. However these methods need to be modified in order to incorporate the spatial dependence of mass. Same as the constant mass systems, the traditional way of obtaining the exact solutions to PDEM systems is to solve the corresponding Schrödinger equation. Several authors have added valuable contributions in this context [35–39].
Schrödinger equation of the corresponding system can be solved by using transformation technique, known as Coordinate transformation method [40]. When position dependent effective mass system is under consideration, the kinetic energy term has

several definitions due to incompatible nature of position and momentum operators. By following von Ross ordering [17, 18], position dependent effective mass Schrödinger equation becomes,

$$\frac{d^2\psi}{dx^2} - \frac{m'(x)}{m(x)}\frac{d\psi(x)}{dx} + 2m[E - V(x)]\psi(x) = 0. \tag{1.2.1}$$

The coordinate transformation method transforms the position coordinate x into new coordinate y i.e., $x \longrightarrow y$. By using Sturm Liouville approach, following coordinate transformation is performed

$$\psi(x) = \sqrt[4]{m(x)}\phi(y), \tag{1.2.2}$$

and

$$y(x) = \int \sqrt{m(x)}dx, \tag{1.2.3}$$

The edge of using coordinate transformation method is that first derivative term disappears so Schrödinger equation becomes simplified whose solutions are well known.

1.3 Construction of Wave Packet

In classical mechanics equation of motion is used to describe the position and momentum variables and these variables are used to determine the state of the system. But in quantum mechanics to study the dynamical behavior of a wave packet, there is need to construct its wave packet, which describes the position and momentum of a particle. A localized wave packet can be produced in many physical systems. A well localized wave packet is a linear superposition of its eigenfunctions at some initial time $t = 0$,

$$\psi(x, 0) = \sum_n c_n u_n(x). \tag{1.3.1}$$

The wave packet displays a variety of non-classical effects. These effects can be observed through several interesting phenomena like fractional revivals, quantum revivals and super revivals of the wave packet at some particular instant of time. Moreover, the physical interpretation of wave packet lies in its modulus square that

provides us with probability density of finding the particle at position x at time t. This wave function is representing a particle which is equally probable to be found anywhere on the x-axis at all times.

1.4 Quantum dynamics of wave packet

The dynamics of wave packets of highly excited states of atoms and molecules and discussion of quantum revivals and fractional revivals of wave packet including experimental observations have been studied in twentieth century i-e in 1991. After progressing in this field many quantum concepts which were hidden behind quantum revivals start to appear. So the study of revival behavior become more interesting to get a review of short and long term quantum revivals of wave packets. The study of revival phenomena [41] can be understand by transition from quantum to classical dynamics and the departure from classical prognostications that are presented during the long term time evolution of wave packet [42]. According to Bohr correspondence principal, for high quantum numbers n$\rightarrow \infty$ the quantum theory regenerates classical mechanics. Quantum to classical transition can be knowing purposeful by decoherence in quantum wave packet. The time evolution of a wave packet and its interactions with boundaries destroy the coherence of wave packet and quantum system gets collapse. The Rydberg wave packets are also used to investigate the correlation between classical and quantum mechanics [43], for the reason that initially the wave packet is moving periodically with classical period same as the charged particle is moving in coulomb field.

The study of localized, time dependent solutions to bound state problems in quantum mechanics is attracting a lot of interest. Schrödinger [44] and others [45] have discussed the wave packet solutions to many familiar problems.

Despite Schrödinger's hope that "wave groups can be constructed which move round highly quantized Kepler ellipses and are the representations by wave mechanics of the hydrogen electron..... " [46] (without spreading,as with the constant width harmonic oscillator packet he derived). From the early exploration it is found that such dispersion [47] was a natural characteristic of wave packet for coulomb potential. On Schrödinger's suggestions, trials for the semi-classical solutions of the

Coulomb problem were continued. Advanced experimental technique such as laser induced excitation of Rydberg wave packets, and other techniques to produce and monitor the time development of such states which developed more interest in wave packets. This interest became the path to new features in the long term time development in such bound state systems, such as quantum wave packet revivals. Parker and Stroud [48–51] were the first to observe this behavior in Rydberg atoms.

The phenomenon of wave packet revivals arises when a well localized wave packet is produced, which travels with time evolution with almost classical periodicity (T_{cl}) and then spreads significantly, different waves travel with different phase, after a number of orbits entering the so called collapsed phase. The initial wave packet, on a large time scale re-localizes it self in the form of quantum revivals, this time is called revival time ($T_{rev} >> T_{cl}$). Additional temporal structures with smaller periodicities are observed. These "mini-packets" are found at times equal to rational fractional of revival time $p/q(T_{rev})$. These "mini-fractions" or "clones" are called fractional revivals [52]. Fractional revivals have been observed in many atomic and molecular systems [53].

1.5 Outline of thesis

In second chapter, we study the quantization of position dependent mass system by replacing the classical observables with their corresponding operators. Then discuss the order ambiguity which appears in kinetic energy term due to presence of incompatible operators and formulate the Schrödinger equation for PDEM quantum Hamiltonian.

In chapter three, we solve the Schrödinger equation of position dependent mass in infinite square well with differnt choices of mass functions. Then further three cases are discussed in which mass increases linearly and abruptly. In the last section of this chapter general expression for increasing mass is derived.

In fourth chapter, We explore the wave packet dynamics by means of autocorrelation and temporal evolution of probability density of spatial wave packet−spatio-temporal dynamics. The image plots of temporal evolution of position-space probability density, known as quantum carpets, are presented to explore the structure

of quantum revivals and fractional revivals. It is found that structure of fractional revivals is modified due the spatially varying mass.

Finally, we present the summary and conclusions of our work in chapter 5.

Chapter 2

Quantization of Position Dependent Effective Mass System

As discussed in introductory chapter, the position dependent effective mass system (PDEM) has vast applications in various areas of physics which have attracted interdisciplinary interests of researchers. However, quantum mechanical description of such systems encounter several mathematical and conceptual difficulties of fundamental nature. In this chapter we will discuss the quantization of PDEM systems and associated issues.

The chapter is organized as follow. In section (2.1), we present classical Hamiltonian that governs the dynamics of classical PDEM system as pre-requisite of quantum dynamics. In section (2.1), various quantization techniques are reviewed which leads to non-equaivalent quantum Hamiltonians with same classical analogue. In section (2.3), we present the resulting Schrödinger equation for general PDEM systems. Finally in section (2.4), we present the conclusion of the chapter.

2.1 Classical dynamics of PDEM systems

The classical dynamics of a system can be described by either of the three equivalent formalisms, namely, Newtonian mechanics, Lagrangian mechanics and Hamiltonian mechanics. As a pre-requisite to the analogous quantum description, discussed in

next section, we present here the derivation of classical Hamiltonian from Lagrangian of the PDEM system.

The Lagrangian of a particle with spatially varying mass $m(x)$ moving in a one-dimensional bounded potential $V(x)$ can be expressed as

$$\mathcal{L}(x, \dot{x}) = \frac{m(x)\dot{x}^2}{2} - V(x). \tag{2.1.1}$$

From the Lagrangian (2.1.1), we can define the momentum of the dynamical system as

$$p = \frac{\partial \mathcal{L}}{\partial \dot{x}} = m(x)\dot{x}. \tag{2.1.2}$$

Now the classical Hamiltonian of the system can be obtained as

$$H(x, p) = p\dot{x} - \mathcal{L} = \frac{p^2}{2m(x)} + V(x), \tag{2.1.3}$$

where we have substituted the value of $\dot{x}$ from Eq. (2.1.2) to obtain the Hamiltonian (2.1.3) in terms of momentum. It is well known fact that in constant mass systems, the kinetic energy term in classical Hamiltonian is only a function of momentum variable. However, it is important to note that in the case of PDEM systems, the kinetic energy term of Hamiltonian (2.1.3) also depends on position in addition to momentum variable. This fundamental difference in the structure of classical Hamiltonian plays an important role in the analogous quantum description of the PDEM systems.

2.2 Quantization of PDEM Hamiltonian

It is well known that generically the classical Hamiltonian is a function of position and momentum variables. As discussed above in section (2.1), in the case of constant mass systems, the kinetic and potential energy terms are respectively the functions of momentum p and position x variables only. While quantizing such classical Hamiltonians, the variables x, p are replaced by their corresponding non-commuting quantum operators $\hat{x}, \hat{p}$, such that $[\hat{x}, \hat{p}] = i\hbar$.

As given in Eq. (2.1.3), the kinetic energy term

$$T(x, p) = \frac{p^2}{2m(x)}, \tag{2.2.1}$$

is a function of both potential and momentum variables, in contrast to the constant mass systems. Therefore, the quantization of position-dependent effective mass systems encounter an ordering ambiguity in placing position-dependent mass $m(\hat{x})$ operator and momentum operator $\hat{p}$ due to incompatible nature of position and momentum operators $\hat{x}, \hat{p}$. In other words, for a generic PDEM system the quantizations of kinetic energy term, given in Eq. (2.2.1), using different orderings is non-equivalent, i.e.,

$$\hat{p}^2 \frac{1}{m(\hat{x})} \neq \frac{1}{m(\hat{x})} \hat{p}^2, \tag{2.2.2}$$

which leads to non-equivalent quantum Hamiltonians. In order to circumvent this issue, several specific ordering methods exist in literature which provide us with non-equivalent quantum Hamiltonian (but same at classical level) of the position dependent effective mass system. In the following we review the most commonly used ordering methods and their resulting quantum Hamiltonians.

The most general and commonly used approach is introduced by Oldwig von Roos [17, 18] which is given as

$$\hat{T} = \frac{1}{4}(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma} + m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha}), \tag{2.2.3}$$

where α, β and γ are arbitrary real constants which satisfy $\alpha + \beta + \gamma = -1$. Several choices for the parameters are suggested in the literature. Among the most famous are given by the Gora and Williams ($\beta = \gamma = 0, \alpha = -1$), Zhu and Kroemer ($\alpha = \gamma = -\frac{1}{2}, \beta = 0$) [20] and Li and Kuhn($\beta = \gamma = \frac{-1}{2}, \alpha = 0$) [19]. Different choices of parameters α, β and γ generate different Hamiltonians.

Keeping in view the invariant Galilean transformations and Hermiticity of the resulting Hamiltonian, Levy-Leblond [21] suggested that a particular choice of these ambiguity parameters with values given as ($\alpha = \beta = 0$) and $\gamma = -1$ gives rise a symmetric ordering

$$T(\hat{x}, \hat{p}) = \frac{1}{2}\hat{p}\frac{1}{m(\hat{x})}\hat{p}, \tag{2.2.4}$$

which leads to a Hermitian quantum Hamiltonian. In our later discussion we will follow this symmetric ordering approach to obtain the quantum Hamiltonian for our position-dependent effective mass systems.

2.3 Schrödinger Equation for PDEM system

Following the Levy-Leblond approach [21], the quantum Hamiltonian of the PDEM system is expressed as

$$H(\hat{x},\hat{p}) = \frac{1}{2}\hat{p}\frac{1}{m(\hat{x})}\hat{p} + V(\hat{x}). \tag{2.3.1}$$

Using position representation of momentum operator, the Schrödinger equation in the configuration space, corresponding to Hamiltonian (2.3.1), is given as

$$\frac{-1}{2}\frac{d}{dx}[\frac{1}{m(x)}\frac{d\psi(x)}{dx}] + V(x)\psi(x) = E\psi(x). \tag{2.3.2}$$

The solutions of this equation depends on the particular choices of $m(x)$ and $V(x)$. However, if $m(x)$ is a bounded but possibly discontinuous function then the wave function $\psi(x)$ should be continuous across the mass discontinuity and at the interface such that

$$\frac{1}{m(x)}\psi'(x)|_{+} = \frac{1}{m(x)}\psi'(x)|_{-}, \tag{2.3.3}$$

where the prime denotes a derivative with respect to the position variable x. In the next chapter we will discuss the solutions of this Schrödinger equation for various choices of consider $m(x)$ and $V(x)$.

2.4 Conclusions

In this short chapter, we have reviewed various quantization techniques for position-dependent effective mass systems. It is found that various orderings of momentum operator and spatially varying mass operator lead to non-equivalent quantum Hamiltonian for the same classical Hamiltonian. In our analysis, we choose Levy-Leblond's [21] symmetric ordering approach which results in the Hermitian Hamiltonian. Finally write the Schrödinger equation for general $m(x)$ and $V(x)$.

Chapter 3

Solutions of Position Dependent Effective Mass Schrödinger Equation

Finding the solutions of Schrödinger equation corresponding to a quantum mechanical system is one of the most important tasks in wave mechanics. For constant mass systems, the solutions of this equation depend on the nature of the bounding potential of the system. The analytical solutions can only be obtained for a limited number of systems and generally it is not possible to solve it for arbitrary potentials. Although numerical techniques are available to obtain the solutions up to very high accuracy, even then analytic solutions are advantageous in many accounts. On the other hand, finding the solutions of position-dependent effective mass systems exhibit greater mathematical difficulty because it depends on the bounding potential as well profile of position-dependence of mass. In this chapter, we present solutions of PDEM system with different variations of mass with position.

Earlier one dimensional Schrödinger equation with position-dependent mass has been solved by several authors [54, 55]. Through point canonical transformation method, Schrdinger equation was written as usual one, which has constant mass. Then for position dependent mass i-e $m = m(x)$ eigenfunctions and eigenvalues can be found analytically by solving Schrödinger equation. Such systems are motivated

by their applications. In both sections, different mass values are considered and their respective Schrödinger equations are solved. The usefulness of coordinate transformation method lies in the fact that in this way first order derivative term vanishes and equation becomes more simplified.

3.1 PDEM particle in infinite square well

The quantum Hamiltonian of a particle with position-dependent effective mass trapped in an infinite square well can be written as

$$H(\hat{x},\hat{p}) = \frac{1}{2}\hat{p}\frac{1}{m(\hat{x})}\hat{p} + V(\hat{x}). \tag{3.1.1}$$

By using this Hamiltonian the Schrödinger equation can be expressed in the following way

$$\frac{-1}{2}\frac{d}{dx}[\frac{1}{m(x)}\frac{d\psi(x)}{dx}] + V(\hat{x})\psi(x) = E\psi(x). \tag{3.1.2}$$

This equation cannot be solved without specifying $m(x)$ and $V(x)$. In infinite square well, $V(\hat{x}) = 0$ for $0 < x < L$ and $V(\hat{x}) = \infty$ otherwise.

$$\frac{-1}{2}\frac{d}{dx}[\frac{1}{m(x)}\frac{d\psi(x)}{dx}] = E\psi(x). \tag{3.1.3}$$

For the qualitative understanding of any quantum system, we need to find its exact solutions, i.e., its eigenfunctions and eigenenergies. The exact solutions can be find out by solving the Eq.(3.1.3). We reparameterize the equation by using the following transformation,

$$\psi(x) = m(x)^{\frac{1}{4}}\phi(y(x)), \qquad \frac{dy}{dx} = m(x)^{\frac{1}{2}}, \tag{3.1.4}$$

which simplifies the above differential equation. However, in order to get the solutions we first need to specify the position dependence of $m(x)$. As a preliminary case, we consider the following form of mass i.e.,

$$m(x) = \frac{m_0}{(\tau x + a)^2}, \tag{3.1.5}$$

where m_0 is a constant mass, which we consider to be 1, τ is a parameter which measures the extent to which mass is depending on position. In this case mass is

inversely related with position. The resulting transformations, given in Eq. (3.1.4) take the form as,

$$\psi(x) = \frac{1}{(\tau x + a)^{\frac{1}{2}}}\phi(y(x)), \qquad \frac{dy}{dx} = m(x)^{\frac{1}{2}} = \frac{1}{(\tau x + a)}. \tag{3.1.6}$$

Using transformations, we get the following differential equation

$$-\frac{1}{2}\frac{d^2\phi(y)}{dy^2} + \frac{\tau^2\phi(y)}{8} = E\phi(y). \tag{3.1.7}$$

This is ordinary second order differential equation whose solutions are well recognized. By solving this equation and applying boundary conditions we get the normalized eigenfunctions and eigen energies,

$$\psi_n(x) = \sqrt{\frac{2\tau}{(1+\tau x)\ln(1+\tau L)}}\sin(\frac{n\pi\ln(1+\tau x)}{\ln(1+\tau L)}), \tag{3.1.8}$$

and the corresponding energy eigenvalues are given as

$$E_n = \frac{\tau^2}{8} + \frac{n^2\pi^2\tau^2}{2\ln^2(1+\tau L)}. \tag{3.1.9}$$

The details of this solution are given in Appendix A at the end of this thesis.

3.1.1 Probability density of eigenstates

By knowing the eigenfunctions of a system, probability density $\rho(x) = |\psi(x)|^2$ of the particle inside the square well can be determined. Comparison between probability densities of position dependent effective mass and constant mass systems explains the unique behavior of PDEM system. In Fig. 3.2, we present the comparison between constant mass and position dependent effective mass by plotting their probability densities versus $X = \frac{x}{L}$ for the first four eigenstates for $\tau = 5$. The purpose of using the larger value of position dependence strength parameter τ is to observe the consequence of spatial dependence on PDEM system. By increasing the strength of position dependence, probability density peaks get more shifted towards higher values of mass and this time shift in the peaks is more prominent.

3.2 Increasing mass with position

In this section taking the same system, namely position dependent effective mass system and the particle confined inside an infinite potential well we consider the interesting case of position dependent effective mass which is increasing with position. The increasing mass case can be interesting in the light of new materials and in abrupt heterostructures.

Let's consider the general case where mass is increasing with position, representing the order of position as x^α. In this case, position dependent mass can be represented in a general form as,

$$m(x) = \frac{x^\alpha}{\tau^2}, \tag{3.2.1}$$

where $\alpha \neq -2$, by using the same transformation method, we can write

$$\psi(x) = m(x)^{\frac{1}{4}}\phi(y(x)) = \frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\phi(y(x)), \tag{3.2.2}$$

$$\frac{dy}{dx} = m(x)^{\frac{1}{2}} = \frac{x^{\frac{\alpha}{2}}}{\tau}, \tag{3.2.3}$$

by re-parameterizing and doing some mathematical steps the differential equation becomes,

$$\frac{-1}{2}\frac{d^2\phi}{dy^2} + \frac{\alpha(3\alpha+4)}{8(\alpha+2)^2y^2}\phi(y) = E\phi(y), \tag{3.2.4}$$

and the solutions of this equation are find out to be,

$$\phi(y) = B_n\sqrt{y(x)}J_\beta(\sqrt{2E_n}y(x)). \tag{3.2.5}$$

where B_n is a normalization constant and $\beta = \frac{(1+\alpha)}{(2+\alpha)}$. Eigenvalues are given in zeros, z_n, of Bessel functions, despite the fact we do not know about an exact expression of zeros, z_n, of Bessel function. Such dependence $m(x) \propto x^n$ can model Heterostructures, both abrupt and smooth one. For abrupt ones, the value of $\alpha = 2$ and $\alpha = 4$ while for smooth ones $\alpha = 1$. For the value of $\alpha = 1$, we can write the solutions by using general solution.

$$\phi(y) = B_n\sqrt{y(x)}\ J_\beta(\sqrt{2E_n}y(x)), \tag{3.2.6}$$

where B_n is a normalization constant and $\beta = \frac{2}{3}$, and eigen energies comes out to be,

$$E_n = \frac{9z_n^2}{8m_0L^3}. \tag{3.2.7}$$

Similarly for the other two values of α we can find the solutions as well. Detailed steps for the solution of general case of increasing mass systems is provided in Appendix B at the end of thesis.

3.3 Conclusions

In this chapter we have solved the Schrödinger equation for a PDEM particle trapped in an infinitely deep square well for two type of masses i.e., one type where mass is inversely related with position and the second one where mass is directly related with position. We obtained the analytic expressions for eigenfunctions and energy eigenvalues. These solutions will be used to explore the wave packet dynamics in PDEM infinite square well in the next chapter. We also explored the comparison between the constant mass system and position dependent effective mass system with the help of probability density plots.

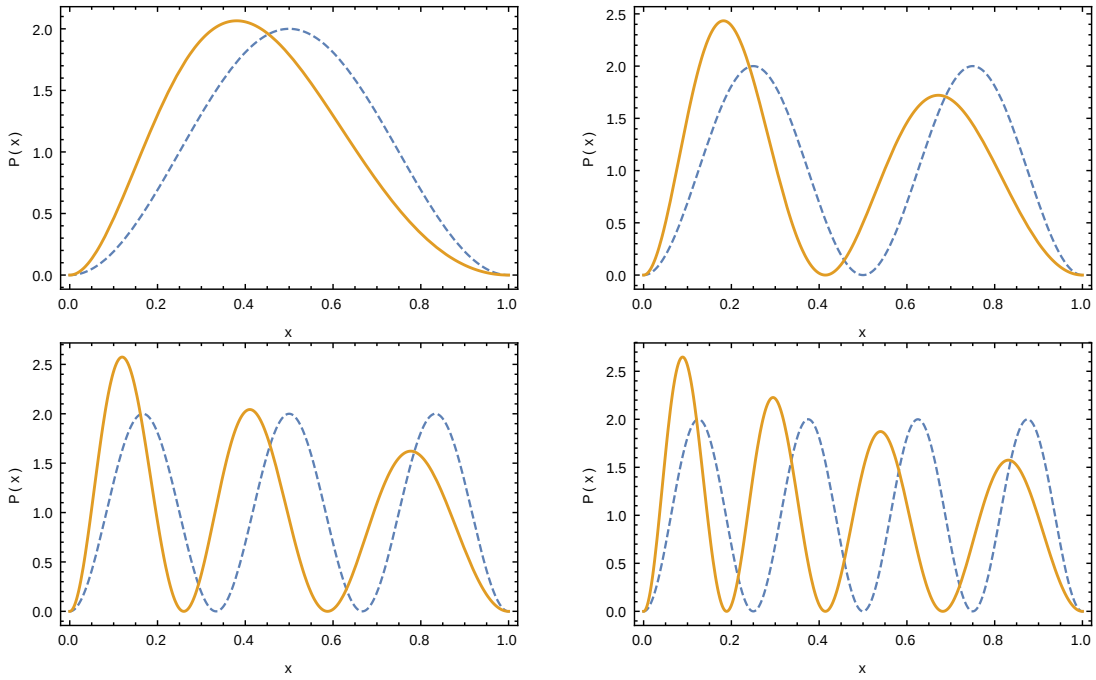

Figure 3.1: Probability density $P(x) = |\varphi_n(x)|^2$ for first four eigenstates vs $X = x/L$: $\tau = m_0 = \hbar = 1$; dashed line for constant mass and solid line for PDEM.

In Fig. 3.1, we present the comparison between constant mass and position dependent effective mass systems by considering their probability densities for first four eigenfunctions i.e., for $n = 1, 2, 3$ and 4. As from the plots, we can observe that probability densities for constant mass system are symmetric while for position dependent effective mass system, they are asymmetric. Moreover, we observe that for position dependent effective mass case, the probability densities are shifted towards higher values of mass (towards lower values of x).

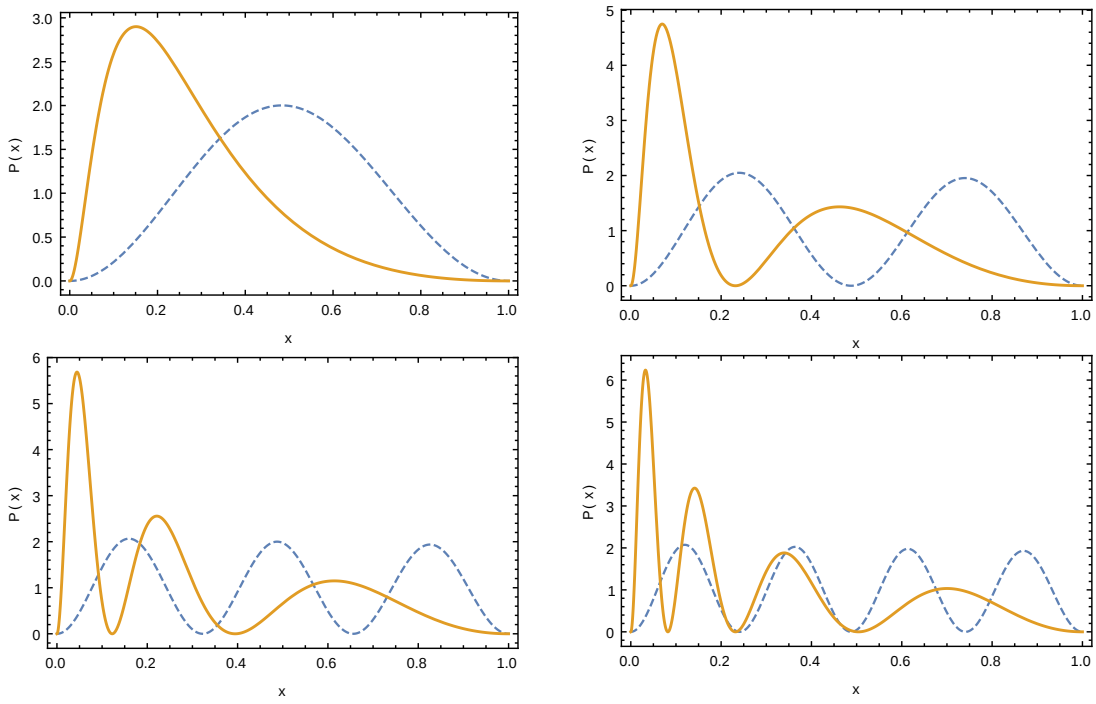

Figure 3.2: Probability density $P(x) = |\varphi_n(x)|^2$ for first four eigenstates vs $X = x/L$: $m_0 = \hbar = 1$; and $\tau = 5$, dashed line for constant mass and solid line for PDEM.

Chapter 4

Wave Packet Dynamics and Quantum Revivals

In bounded dynamical systems, the wave packet evolution manifests recurrences at different time scales, such as, classical periodicity, quantum revivals, super-revivals and fractional revivals. The phenomena was predicted in many physical systems with nonlinear energy spectrum and have been observed experimentally in many systems such as Rydberg wave packets in atomic systems. This phenomenon occurs when an initially well localized wave packet evolves in time in a bounded system. In its early short term time evolution, it follows classical trajectory with periodicity T_{cl} equivalent to its classical time period. Later on it spreads due to dephasing between constituent eigenstates of the superposition and observes a collapse when destructive interference dominates. After a particular period of time the wave packet re-localizes itself when constituent eigenstates attain the initial phase and constructive interference dominates. This time required for re-localization is called quantum revival time T_{rev}. In addition to the full revivals, fractional copies of the original wave packet appears at various fractions of revival time, i.e., $p/q(T_{rev})$ where p, q are relative prime numbers.

In this chapter, we study wave packet dynamics for a particle with spatially varying mass, such that mass is inversely related with position as given by Eq.(3.1.5), trapped in an infinitely deep potential well. We explore the phenomena of quantum revivals and fractional revivals by means of autocorrelation function and temporal

evolution of position-space probability density. It is found that structure of fractional revivals is modified due to the spatially varying mass.

4.1 Time evolution of a wave packet

The dynamics of a quantum mechanical system is governed by its corresponding Hamiltonian

$$\hat{H} = \frac{\hat{p^2}}{2m} + V(\hat{x}). \tag{4.1.1}$$

More explicitly, a wave packet is constructed by a linear superposition of the eigenstates of Hamiltonian (4.1.1) given as,

$$\psi(x,0) = \sum_{n=0}^{\infty} c_n u_n(x), \tag{4.1.2}$$

where $u_n(x)$ is the nth eigenstate of Hamiltonian (4.1.1) and c_n is the corresponding probability amplitude in superposition (4.1.2). For a given initial wave packet in position space and known eigenstates of a given system, the probability amplitudes can be calculated as,

$$c_n = \int_{-\infty}^{\infty} \psi(x,0) u_n^*(x) dx, \tag{4.1.3}$$

where $u_n^*(x)$ is complex conjugate of $u_n(x)$. In our later discussion we will consider the initial wave packet $\psi(x,0)$ as a Gaussian centered at x_0, defined as,

$$\psi(x,0) = \frac{1}{(\sigma\pi^2)^{\frac{1}{4}}} \exp(\frac{-(x-x_0)^2}{2\sigma^2}) \exp(\frac{ip_0 x}{\hbar}), \tag{4.1.4}$$

where p_0 is the initial momentum and σ is the spread of the wave packet at FWHM.

The time evolution of the initial wave packet is governed by the time evolution operator $U(t) = \exp(-iHt/\hbar)$ such that

$$\psi(x,t) = U(t)\psi(x,0) = \sum_{n=1}^{\infty} c_n u_n(x) \exp(\frac{-iE_n t}{\hbar}), \tag{4.1.5}$$

where E_n is the energy eigenvalue corresponding Hamiltonian (4.1.1). It is important to note that the temporal evolution of a wave packet explicitly depends on the structure of the energy spectrum of the system. This dependence is discussed in the next section.

4.2 Quantum revivals and fractional revivals

The time development of the wave packet $\psi(x,t)$, given in Eq. (4.1.5), depends on the phases $\exp(-iE_nt/\hbar)$ which in turn depends on the structure of the energy spectrum E_n of the system. It is well known fact that wave packet follows classical-like evolution if energy spectrum E_n is linear in quantum number n, as in the case of harmonic oscillator. However, if the energy spectrum is nonlinear in n, the wave packet undergoes classical-like evolution only for a few classical periods after which nonlinear dephasing dominates and wave packet observes the phenomena of collapse and revivals.

For a well localized wave packet excited with spread $\triangle n$ around a large central quantum number n_0, such that $n_0 >> \triangle n >> 1$, we can expand E_n by Taylor series about n_0 as,

$$E_n = E_{n_0} + \sum_{r=1}^{\infty} \frac{1}{r!} \frac{d^r E_n}{dn^r}\bigg|_{n=n_0} (n-n_0)^r \,. \tag{4.2.1}$$

Substituting the expansion (4.2.1) in the phase factor $\exp(\frac{-iE_nt}{\hbar})$, we get

$$\exp\left(\frac{-iE_nt}{\hbar}\right) = \exp\left(\frac{-it}{\hbar}\left[E(n_0) + (n-n_0)E'(n_0) + \frac{(n-n_0)^2}{2}E''(n_0) + ...\right]\right), \tag{4.2.2}$$

where $E'(n_0)$ is derivative of E_n with respect to n at $n = n_0$. It is important to note that the first term of the expansion produces a universal phase factor and do not contribute to the dynamics of the wave packet. However, each of the successive terms define a characteristic time scale of periodicity given as

$$T_{(r)} = 2\pi \left(\frac{1}{r!}\frac{\partial^r E_n}{\partial n^r}\bigg|_{n=n_0}\right)^{-1}, \tag{4.2.3}$$

such that $T_1 < T_2 < T_3$, where, $T_{(1)} = T_c$ is the classical period, $T_{(2)} = T_{rev}$ is the quantum revival and $T_{(3)} = T_{sup}$ is the super-revival time.

In our following discussion we will consider the wave packet evolution in the infinite square well. Since its energy spectrum is quadratic in quantum number, therefore the wave packet evolutions exhibit only the classical periodicity and quantum revivals and all the higher order recurrences would be absent. Using the value of E_n from Eq.(4.2.2), in Eq. (4.2.3) and taking the derivatives, the values of classical

period $T_{cl} = 2mL^2/n_0\hbar\pi$ and quantum revival time $T_{rev} = 4mL^2/\hbar\pi$ for constant mass system.

In addition to the complete revival of the wave packet, fractional revivals of various order appear at times $t = T_{rev}p/q$, where p, q are mutually prime numbers. Complete mirror symmetry exists in the structure of fractional revivals about $t = T_{rev}/2$. Therefore, in order to analyze the fractional revivals we consider a time period equal to $T_{rev}/2$. If the eigen energy of a system is known, then classical time period and quantum time period can be determined by using Eq.(4.2.3). For constant mass system classical and quantum revival time comes out to be
$T_{cl} = \frac{2mL^2}{n_0\pi\hbar}$ and $T_{rev} = \frac{4mL^2}{\pi\hbar}$.
Similarly eigen energy for PDEM provided in Eq.(3.1.9) helps out to find classical and revival time for this system,
$T_{cl} = \frac{2\ln^2(1+L)}{n_0\pi\hbar\tau^2}$ and $T_{rev} = \frac{4\ln^2(1+L)}{\pi\hbar\tau_2}$.

T_{cl} and T_{rev} of PDEM system is less than T_{cl} and T_{rev} of constant mass respectively. But $\frac{T_{rev}}{T_{cl}} = 2n_0$ is same in both systems because T_{rev} and T_{cl} reduces with the same rate. The quantum revival occurs after the same number of classical periods in PDEM as in constant mass system.

4.3 Measures on quantum revivals and fractional revivals

In order to characterize the temporal evolution of the wave packets, some quantitative measures are required. In this section, we explore various analytic methods to characterize the structure of quantum revivals and fractional revivals during wave packet evolution.

4.3.1 Autocorrelation function

The most commonly used criterion for characterization of wave packet evolution is the autocorrelation function which is an overlap between an initial wave packet and

time-evolved one, that is

$$A(t) = \langle \psi(t) | \psi_0 \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,0)dx, \tag{4.3.1}$$

where $\psi^*(x,t)$ is the complex conjugate of the time evolved wave packet. Using Eqs. (4.1.2) and (4.1.5) in Eq. (4.3.1), we get a simple useful form of autocorrelation function as,

$$A(t) = \sum_{n=1}^{\infty} |c_n|^2 \exp[\frac{iE_n t}{\hbar}]. \tag{4.3.2}$$

The autocorrelation function is important in the study of revival behavior in the pump probe type experiment [56]. Other than theoretical value, autocorrelation function is important in pump probe type experiment, where it is observed experimentally that autocorrelation function is related to the observable ionization signal [57, 58].

The plots of autocorrelation function for the constant mass and position dependent effective mass systems are the same. The Fig. 4.1, represents the modulus square of autocorrelation function versus T where the horizontal axis is rescaled by classical period such that $T = \frac{t}{T_{cl}}$. In this figure plots are shown for $p_0 = 5\pi, 10\pi$, 15π and 20π from top to bottom respectively. The plots show that initially the wave packet was well localized, with time evolution spread in wave packet increases and the constituent waves travel with different phases which results in collapse. After long time evolution, constructive interference takes place and the wave packet relocalizes itself. It is obvious from the plots that the wave packet revival occurs after a smaller (larger) number of classical periods as the value of p_0 is decreased(increased). This is due to the fact that $\frac{T_{rev}}{T_{cl}} = 2n_0$ and $p_n = \frac{n\pi\hbar}{L}$ such that $p_0 = \frac{n_0\pi\hbar}{L}$. For a wave packet with initial momentum, quantum revival occurs after $2n(since \hbar L = 1)$ classical periods.

In addition to complete revival phenomenon, we also observe some fractional revivals at times $t = \frac{p}{q}T_{rev}$. It is obvious from Fig. 4.1, that a complete mirror symmetry exists in the structure of fractional revivals about $t = \frac{T_{rev}}{2}$. Therefore, in order to analyze the fractional revivals, we consider a time period equal to $\frac{Trev}{2}$.

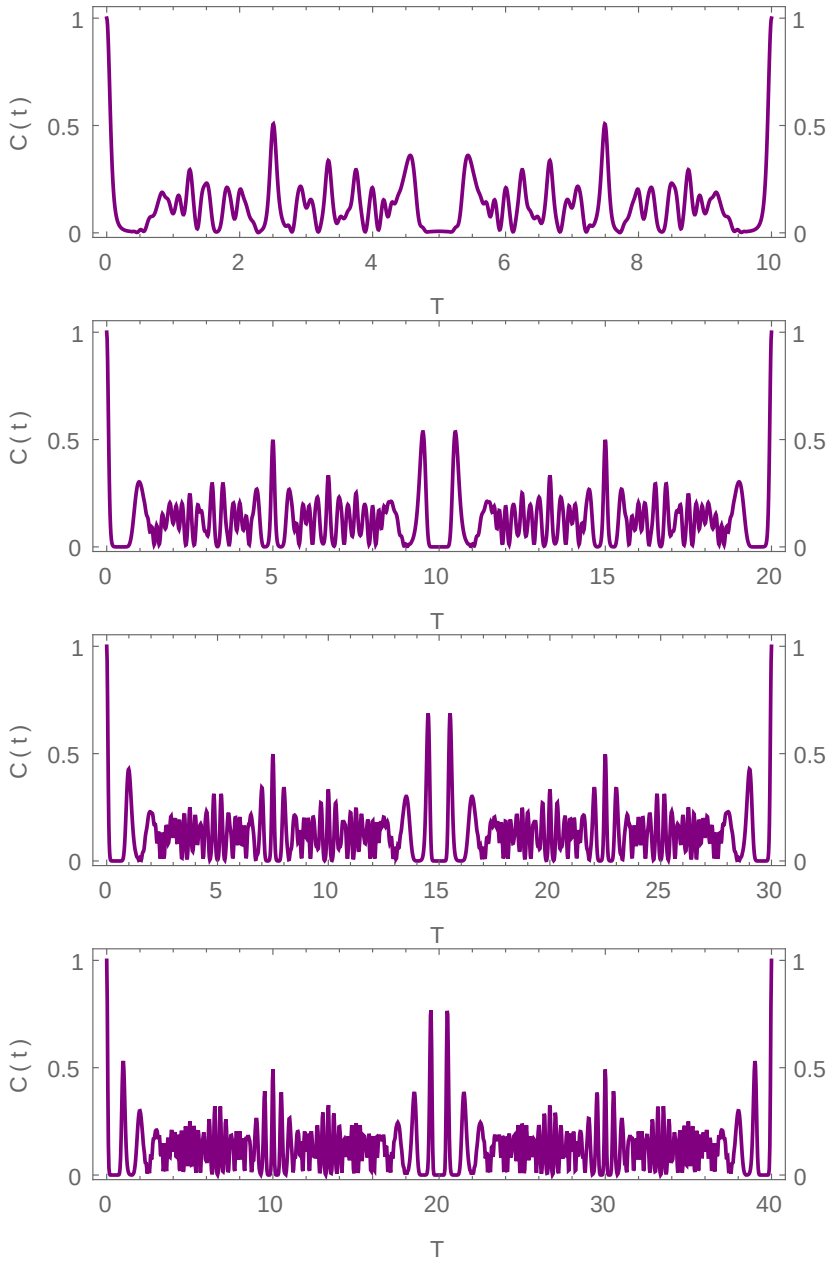

Figure 4.1: The initial evolution of $C(t) = |A(t)|^2$ for an initial Gaussian wave packet of width $\sigma = 0.1$ centered at the middle of the well $x_0 = \frac{L}{2}$ for different values of the initial momentum $p_0 = 5\pi, 10\pi$, 15π and 20π from top to bottom respectively. The $C(t) = |A(t)|^2$ is plotted for one revival time T_{rev}, where the horizontal axis is rescaled by classical period such that $T = \frac{t}{T_{cl}}$.

4.3.2 Spatio-temporal evolution of probability density

Alternatively, the time evolution of a wave packet can be characterized by means of temporal evolution of position-space probability density $\rho(x,t) = |\psi(x,t)|^2$. The dynamics of an initially well localized wave packet undergoes a series of constructive and destructive interferences which leads to the formation of regular interference patterns known as quantum carpets. Quantum carpets appear in many fields of wave physics ranging from quantum mechanics, with application in Bose-Einstein condensation and nuclear physics to electromagnetic waves and wave guide. Quantum carpet is a useful tool for the study of quantum revivals and fractional revivals. In this subsection we present the formation of quantum carpets which can serve as a tool to analyze the structure of fractional revivals.

Using Eq. (4.1.5), we calculate the time evolution of probability density in position space which is as

$$\rho(x,t) = |\psi(x,t)|^2 = \sum_{n,m=0}^{\infty} c_n c_m^* u_n(x) u_m^*(x) e^{-i(E_n - E_m)t/\hbar}. \tag{4.3.3}$$

For our explicit discussion, we will use the energy eigenfunctions and eigenvalues for position-dependent effective mass particle trapped in infinite square well, obtained in previous chapter. Moreover we will compare the results with analogous constant mass system. The resulting quantum carpets are presented in the next section.

Fig. 4.2 shows the probability density of the Gaussian wave packet centered at $x_0 = \frac{L}{2}$ with initial momentum $p_0 = 5\pi$ for constant mass system and position dependent effective mass system for $\tau = 1$ at different values of time: at $t = 0$, $t = T_{rev}/4$, $t = T_{rev}/2$, $t = 3T_{rev}/4$ respectively from top left to bottom right. The probability density for constant mass is represented by dotted line and for position dependent effective mass by solid line. This figure shows that in position dependent case peaks are shifted towards higher values of mass or we can conclude that particle would like to be in those areas of well where mass has higher values.

Fig. 4.3 shows the probability density peaks for constant mass and position dependent effective mass particle at $t = \frac{T_{rev}}{4}$ for different values of position dependence strength parameter $\tau = 0.5$, $\tau = 1.3$, $\tau = 5$, $\tau = 10$ respectively from top left to bottom right to observe the effect of position dependence strength parameter. Due

to position dependence effect, peaks are shifted towards higher values of mass and by increasing the position dependence strength shift in peaks is more prominent. Fig. 4.4 represents the comparison between probability densities of constant mass particle and position dependent mass particle and effect of increasing the position dependence strength parameter at $t = \frac{T_{rev}}{2}$. It can been seen from the figure that peaks of PDEM particle are shifted towards lower values of x where the mass has larger values and for larger values of position dependence strength parameter the shifting in peaks is more prominent.

In Fig. 4.5, we represent the comparison between quantum carpets of constant mass case and position dependent effective mass case with $\tau = 1.3$ from left to right respectively. These quantum carpets are woven by the Gaussian wave packet centered at $x_0 = \frac{L}{2}$ with initial momentum $p_0 = 5\pi$. This Fig. 4.5 shows the time evolution of the position space probability density for a Gaussian wave packet for full revival time, which explains the formation of quantum carpets in the position space. It is obvious from the carpet that a well localized single peaked probability density of the wave packet evolves quasi-classically during its early time evolution and splits into multiple sub-peaks after successive bounces with the walls of the deep square well, where a self-interference of the wave packet takes place. These multiple sub-peaks then evolve in time with their own phases and undergo a series of constructive and destructive interferences. This results in the formation of regular arrangement of maximum probability regions–bright fringes known as ridges and minimum probability regions–dark fringes known as canals. During this course of the time evolution, fractional copies of the original wave packet appear at times $t = \frac{p}{q}T_{rev}$ with p,q being mutually prime numbers. In these plots fractional revivals can easily be observed. Moreover the quantum carpet for the constant mass case (left carpet) is symmetric, that is, probability densities are equally distributed while the quantum carpet for position dependent effective mass case is asymmetric, that is, probability densities are not equally distributed in the well but they are shifted towards left part of the well where the mass has larger values.

In Fig. 4.6, we present the quantum carpets of position dependent effective mass system with $\tau = 5$ and $\tau = 10$ from left to right respectively. These quantum carpets are woven by the Gaussian eave packet centered at $x_0 = \frac{L}{2}$ with initial momentum

$p_0 = 5\pi$. These carpets show the time evolution of the position space probability density for a Gaussian wave packet for full revival time, which explains the formation of quantum carpets in the position space. These carpets show that by increasing the position dependent strength, probability densities of particles shifted towards greater values of mass and it is obvious from these two plots that for larger position dependent strength, shift in the probability density becomes more prominent.

4.4 Conclusions

In this chapter we have studied the autocorrelation function and quantum carpets for initially well localized wave packet evolving in spatially varying mass in infinite square well. It is found that the autocorrelation function can not determine the effect of spatially varying mass. However, by means of quantum carpets it is found that structure of fractional revivals is modified due to the spatially varying mass. In order to understand the effects of spatial-dependence on wave packet evolution, we have compared the results with corresponding constant mass systems and also observe the effect of position dependence strength. This leads us to conclude that spatial-dependence of mass modifies the design of quantum carpets and hence the structure of fractional revivals.

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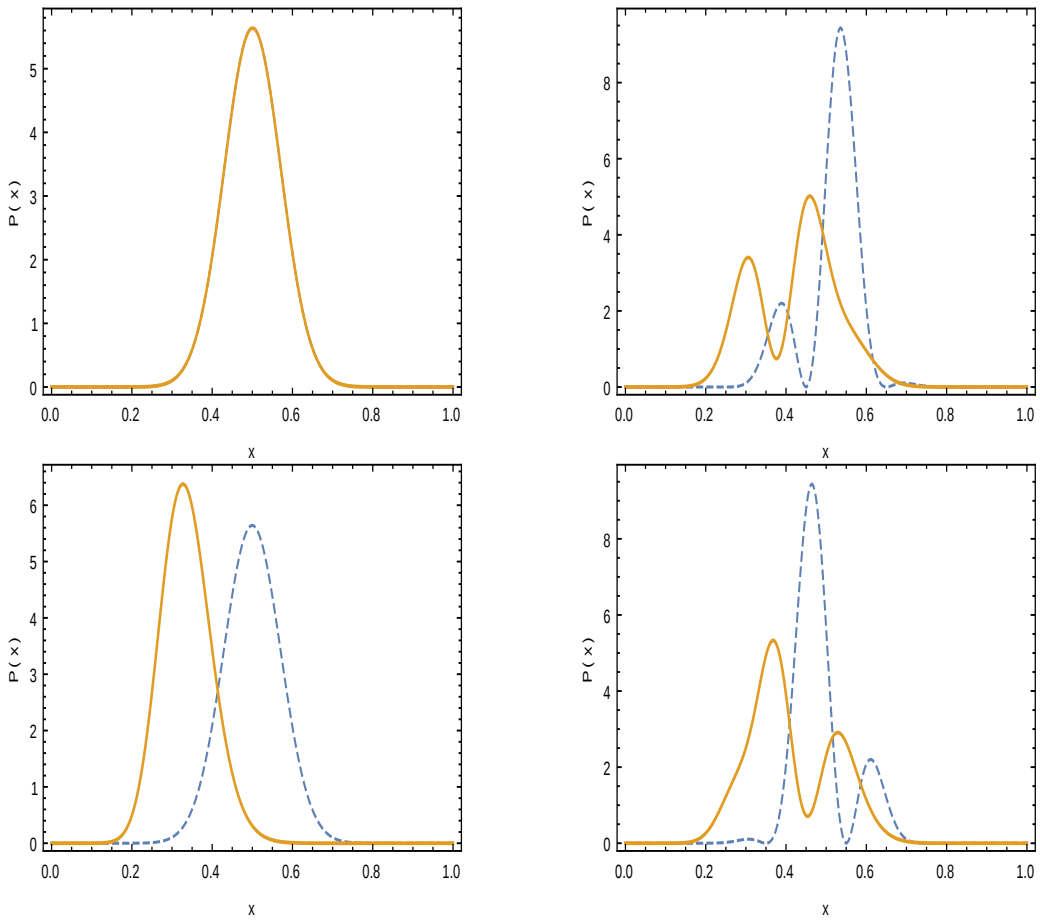

Figure 4.2: Probability density $P(x) = |\psi(x,t)|^2$ of the Gaussian WP centered at $x_0 = L/2$ with initial momentum $p_0 = 5\pi$ vs $X = x/L$ for $\tau = 1$: at $t = 0$, $t = T_{rev}/4$, $t = T_{rev}/2$, $t = 3T_{rev}/4$ from top left to bottom right respectively.

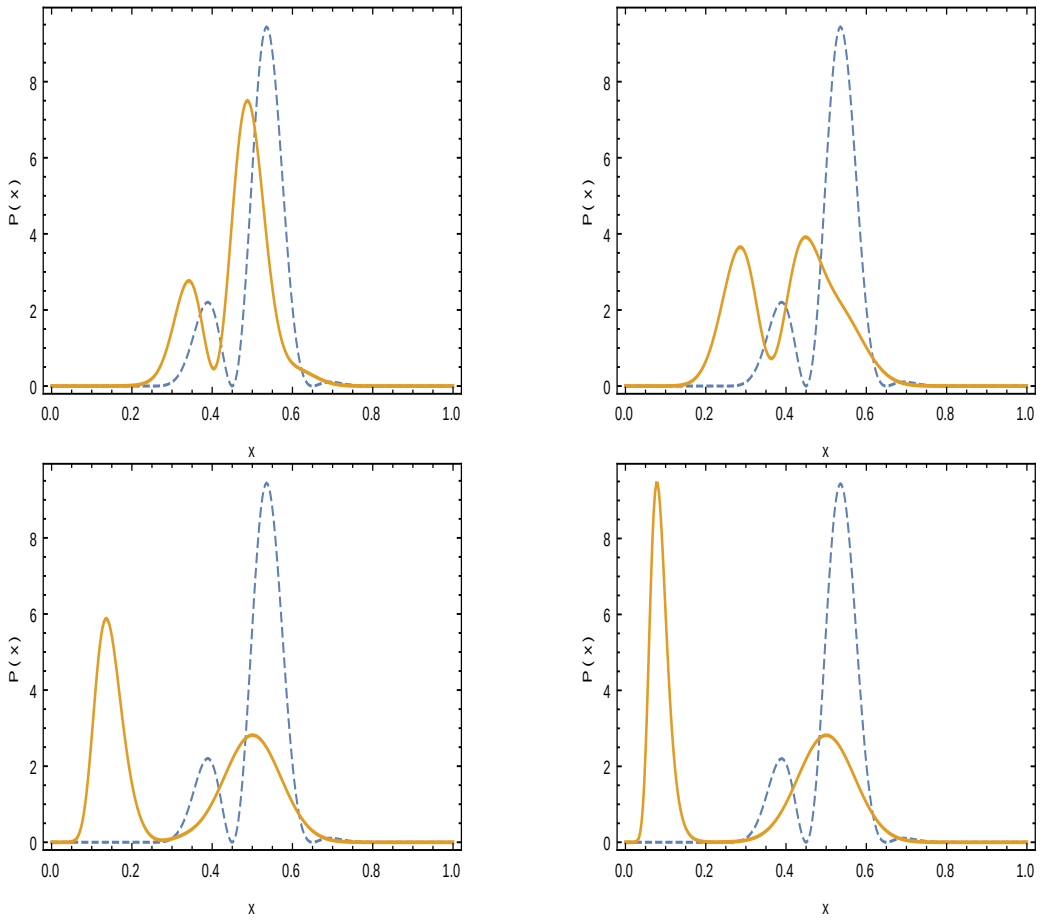

Figure 4.3: Probability density $P(x) = |\psi(x,t)|^2$ of the same WP vs $X = x/L$ at $t = T_{rev}/4$ for different values of τ: $\tau = 0.5$, $\tau = 1.3$, $\tau = 5$, $\tau = 10$ respectively from top left to bottom right.

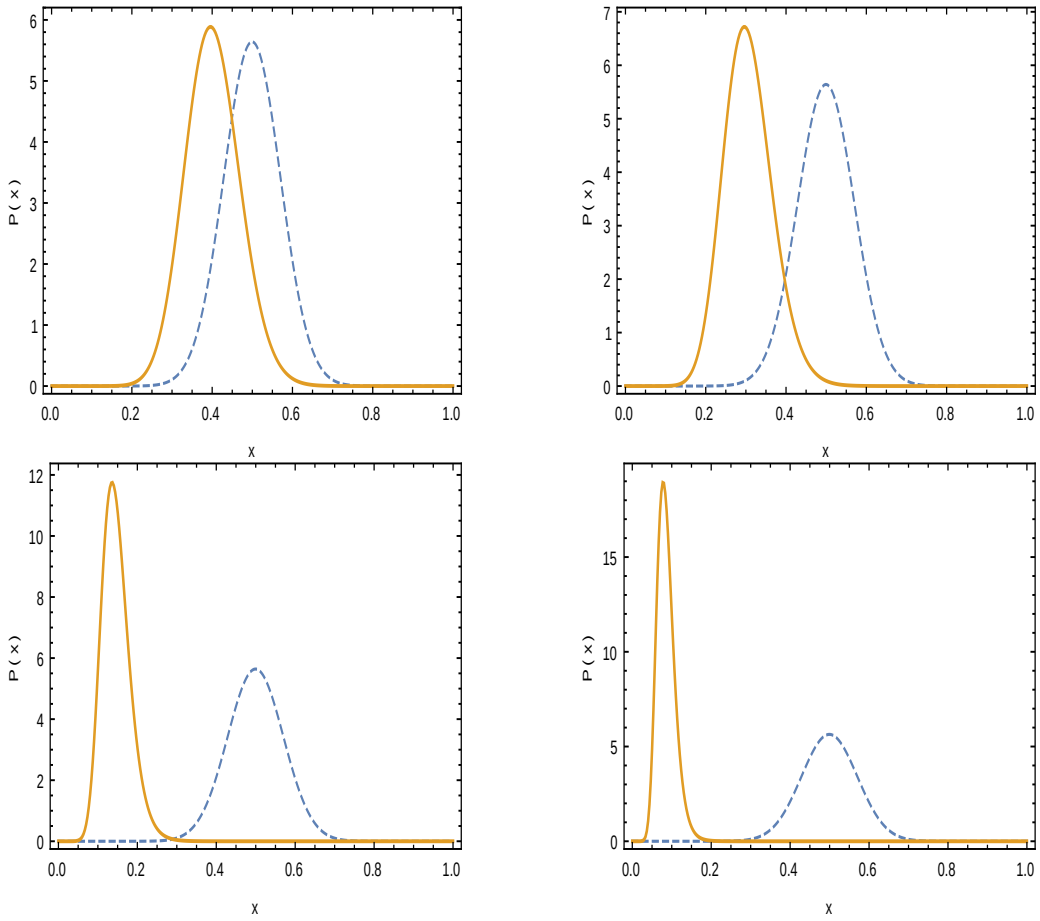

Figure 4.4: Probability density $P(x) = |\psi(x,t)|^2$ of the same WP vs $X = x/L$ at $t = T_{rev}/2$ for different values of τ: $\tau = 0.5$, $\tau = 1.3$,$\tau = 5$,$\tau = 10$ respectively from top left to bottom right.

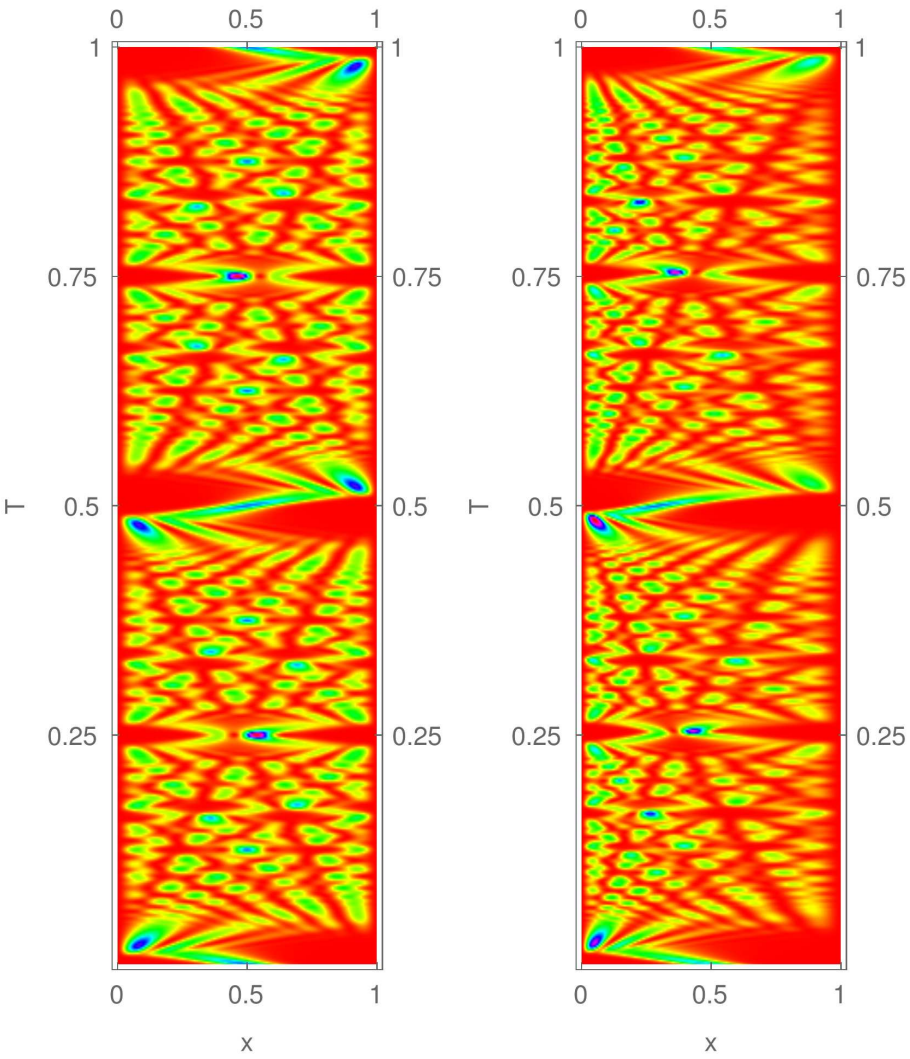

Figure 4.5: Quantum carpets woven by the same Gaussian WP: (from left to right) for constant mass system and PDEM system with $\tau = 1.3$.

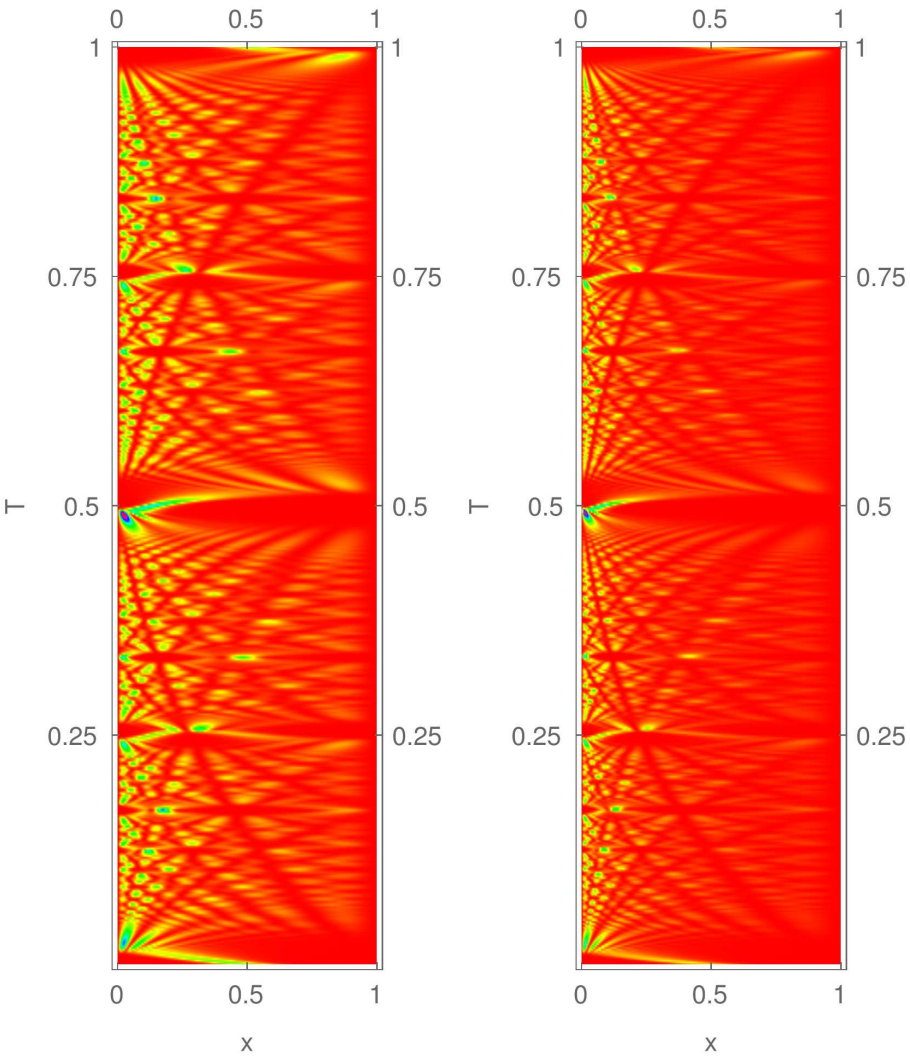

Figure 4.6: Quantum carpets woven by the same Gaussian WP: (from left to right) for PDEM system with $\tau = 5$ and $\tau = 10$ respectively.

Chapter 5

Summary and Conclusion

In this thesis we have studied the position dependent effective mass system. In our work, we discussed the order ambiguity that arises in writing the kinetic Hamiltonian of position dependent effective mass system due to non-commuting nature of position and momentum operators as both are appearing in kinetic term.

We studied the case of position dependent mass particle in infinite square well. We studied its Schrödinger equation and solved it by using coordinate transformation method and boundary conditions to determine its eigen functions and eigen energies. We studied the solutions of another case of position dependent effective mass in which mass is directly increasing with respect to position.

Further we studied the dynamics of wave packet in context of quantum revival. In our work, we studied the general construction of well localized wave packet, which is constructed by superposition of its all possible eigenstates of that system. We studied the time evolution of wave packet and different periodicities. Time evolved state is formed in the result of interaction of an initial state of the system with time evolution operator. We studied the quantum revival behavior by means of considering initially localized wave packet exhibits short term time evolution. With time evolution, wave packet spreads, collapses, reverses and re-localizes. The re-localization of wave packet is called the revival of wave packet. We constructed the probability density as a function of space. We also compared the constant and position dependent mass systems with the help of probability density for different time revivals and the effect of position dependence strength on probability density

peaks. We observed that probability peaks are more shifted towards larger values of mass.

We explored the wave packet dynamics by means of autocorrelation and temporal evolution of probability density of spatial wave packet, spatio-temporal dynamics. We found that revival time for PDM system is less than that for constant mass system. Moreover, we came across the fact that plots of autocorrelation are same for both systems. The image plots of temporal evolution of position-space probability density, known as quantum carpets, are presented to explore the structure of quantum revivals and fractional revivals. In order to understand the effects of spatial-dependence on wave packet evolution, we have compared the results with corresponding constant mass systems. It is found that structure of fractional revivals is modified due to the spatially varying mass such that fractional revivals are shifted towards larger values of mass. This leads us to conclude that spatial-dependence of mass modifies the design of quantum carpets and hence the structure of fractional revivals.

Appendices

Appendix A

Appendix

Solution of PDEM system for $m(x) = \frac{1}{(\tau x+a)^2}$

In this case, mass is inversely related with position. By using the von Ross ordering, quantum Hamiltonian of the PDEM system finds out to be,

$$H(\hat{x}, \hat{p}) = \frac{1}{2}\hat{p}\frac{1}{m(\hat{x})}\hat{p} + V(\hat{x}). \tag{A.0.1}$$

$$\frac{-1}{2}\frac{d}{dx}[\frac{1}{m(x)}\frac{d\psi(x)}{dx}] = E\psi(x). \tag{A.0.2}$$

The exact solutions can be find out by solving the Eq.(3.1.3). We re-parameterize the equation by using the following transformation,

$$\psi(x) = m(x)^{\frac{1}{4}}\phi(y(x)), \qquad \frac{dy}{dx} = m(x)^{\frac{1}{2}}, \tag{A.0.3}$$

and the resulting transformations, given in Eq. (3.1.4) take the form as,

$$\psi(x) = \frac{1}{(\tau x + a)^{\frac{1}{2}}}\phi(y(x)), \qquad \frac{dy}{dx} = m(x)^{\frac{1}{2}} = \frac{1}{(\tau x + a)}, \tag{A.0.4}$$

Using transformations, given in Eq. (A.0.4), in to Eq. (3.1.3) we get differential equation

$$\frac{d\psi}{dx} = \frac{-1}{2}\frac{\tau}{(\tau x + a)^{\frac{3}{2}}}\phi(y(x)) + \frac{1}{(\tau x + a)^{\frac{3}{2}}}\frac{d\phi}{dy}, \tag{A.0.5}$$

$$\frac{-1}{2}\frac{d}{dx}[\frac{1}{m(x)}\frac{d\psi(x)}{dx}] = E\psi(x), \tag{A.0.6}$$

substitute the values of $m(x)$ and $\frac{d\psi}{dx}$ from Eq.(A.0.5), then equation will be transformed into new coordinates

$$\frac{-1}{2}\frac{d}{dx}[(\tau x+a)^2\{\frac{-1}{2}\frac{\tau}{(\tau x+a)^{\frac{3}{2}}}\phi(y(x))+\frac{1}{(\tau x+a)^{\frac{3}{2}}}\frac{d\phi}{dy}\}]=E\frac{1}{(\tau x+a)^{\frac{1}{2}}}\phi(y(x)), \tag{A.0.7}$$

doing multiplication to simplify the equation,

$$\frac{-1}{2}\frac{d}{dx}[\frac{-\tau(\tau x+a)^{\frac{1}{2}}}{2}\phi(y(x))+(\tau x+a)^{\frac{1}{2}}\frac{d\phi}{dy}]=E\frac{1}{(\tau x+a)^{\frac{1}{2}}}\phi(y(x)), \tag{A.0.8}$$

solving the second derivative and we get, simplifying the equation and substitute the value of $\frac{dy}{dx}$,

$$\frac{-1}{2}[\frac{-\tau^2}{4}\frac{1}{(\tau x+a)^{\frac{1}{2}}}\phi(y(x))-\frac{\tau}{2}\frac{1}{(\tau x+a)^{\frac{1}{2}}}\frac{d\phi}{dy}+\frac{\tau}{2}\frac{1}{(\tau x+a)^{\frac{1}{2}}}\frac{d\phi}{dy}+\frac{1}{(\tau x+a)^{\frac{1}{2}}}\frac{d^2\phi}{dy^2}], \tag{A.0.9}$$

just rearranging the equation and resultant equation will be like,

$$\frac{-1}{2(\tau x+a)^{\frac{1}{2}}}\frac{d^2\phi}{dy^2}+\frac{\tau^2}{8}\frac{1}{(\tau x+a)^{\frac{1}{2}}}\phi(y(x))=E\frac{1}{(\tau x+a)^{\frac{1}{2}}}\phi(y(x)), \tag{A.0.10}$$

canceling $\frac{1}{(\tau x+a)^{\frac{1}{2}}}$ from both sides,

$$\frac{-1}{2}\frac{d^2\phi}{dy^2}+\frac{\tau^2}{8}\phi(y(x))=E\phi(y(x)), \tag{A.0.11}$$

simplifying the equation,

$$\frac{d^2\phi}{dy^2}=-(2E-\frac{\tau^2}{4})\phi(y(x)), \tag{A.0.12}$$

for the ease of solution we consider the term $2E-\frac{\tau^2}{4}$ equal to some constant k^2.

$$\frac{d^2\phi}{dy^2}=-k^2\phi(y(x)), \tag{A.0.13}$$

this is second order differential equation and solution of this equation is,

$$\phi(y)=A\cos(ky)+B\sin(ky), \tag{A.0.14}$$

to find the value of y, use equation (A.0.4)

$$\frac{dy}{dx}=\frac{1}{(\tau x+a)}, \tag{A.0.15}$$

and by solving the integral, we obtain y in terms of x,

$$y = \frac{1}{\tau}\ln(\tau x + a), \tag{A.0.16}$$

putting this value of $y$in A.0.14,

$$\frac{\psi(x)}{m(x)^{\frac{1}{4}}} = A\cos(k\frac{\ln(\tau x + a)}{\tau}) + B\sin(k\frac{\ln(\tau x + a)}{\tau}). \tag{A.0.17}$$

Boundary conditions are,

$$\psi(o) = \psi(L) = 0, \tag{A.0.18}$$

apply first boundary condition i-e, $\psi(o) = 0$. With the purpose of having an exact solution of the eigen value equation, we choose a=1.

$$\psi(o) = m(x)^{\frac{1}{4}}A\cos(k\frac{\ln(0+1)}{\tau}) + m(x)^{\frac{1}{4}}B\sin(k\frac{\ln(0+1)}{\tau}), \tag{A.0.19}$$

after using first boundary condition we come to know that A should be 0 to satisfy the boundary condition. So, we put

$$A = 0, \tag{A.0.20}$$

remaining part of equation is,

$$\psi(x) = m(x)^{\frac{1}{4}}B\sin(k\frac{\ln(1+\tau x)}{\tau}), \tag{A.0.21}$$

now using second boundary condition i-e, $\Psi(L) = 0$

$$\psi(L) = m(L)^{\frac{1}{4}}B\sin(k\frac{\ln(1+\tau L)}{\tau}) = 0, \tag{A.0.22}$$

as it is obvious that

$$m(L)^{\frac{1}{4}}B \neq 0, \tag{A.0.23}$$

so,

$$\sin(k\frac{\ln(1+\tau L)}{\tau}) = 0, \tag{A.0.24}$$

finding the value of K,

$$k = \frac{n\pi\tau}{\ln(1+\tau L)}, \tag{A.0.25}$$

substitute this value of k in Eq.(A.0.21),

$$\psi_n(x) = m(x)^{\frac{1}{4}} B \sin(\frac{n\pi\tau \ln(1+\tau x)}{\ln(1+\tau L)\tau}). \tag{A.0.26}$$

Here B is normalization constant, need to be determined. We use normalization condition to find the value of B. Normalization condition is defined as,

$$\int_0^L |\psi(x)|^2 dx = 1, \tag{A.0.27}$$

$$\int_0^L \frac{1}{(\tau x + a)} B^2 \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = 1, \tag{A.0.28}$$

$$B^2 \int_0^L \frac{1}{(\tau x + a)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = 1, \tag{A.0.29}$$

from Eq.(A.0.16)

$$y = \ln(1+\tau x), \tag{A.0.30}$$

taking exp on both sides, in order to replace dx by dy,

$$\exp(y) = (1+\tau x), \tag{A.0.31}$$

$$\exp(y)dy = \tau dx, \tag{A.0.32}$$

Let $b = \frac{n\pi}{\ln(1+\tau L)}$ Limits of integration will be changed according to new coordinate,

when $x = 0$ *then* $y = 0$,

when $x = L$ *then* $y = \ln(1+\tau L)$,

now we will use these new integration limits,

$$\int_0^L \frac{1}{(\tau x+1)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = \int_0^{\ln(1+\tau L)} \frac{1}{\tau \exp(y)} \sin^2(by) \exp(y) dy, \tag{A.0.33}$$

$$\int_0^L \frac{1}{\tau(\tau x+1)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = \frac{1}{\tau} \int_0^{\ln(1+\tau L)} \sin^2(by) dy, \tag{A.0.34}$$

using the half angle formula,

$$\int_0^L \frac{1}{(\tau x+1)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = \frac{1}{\tau} \int_0^{\ln(1+\tau L)} (\frac{1-\cos(2by)}{2}) dy, \tag{A.0.35}$$

$$\int_0^L \frac{1}{(\tau x+1)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = \frac{1}{\tau}[\int_0^{\ln(1+\tau L)} \frac{1}{2} dy - \frac{1}{2}\int_0^{\ln(1+\tau L)} \cos(2by) dy], \tag{A.0.36}$$

after solving the integration with limits,

$$\int_0^L \frac{1}{(\tau x+1)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = \frac{1}{\tau}[\frac{1}{2}(\ln(1+\tau L)-0) - \frac{1}{4b}(\sin(\frac{2n\pi \ln(1+\tau L)}{\ln(1+\tau L)})-0)], \tag{A.0.37}$$

$$\int_0^L \frac{1}{\tau(\tau x+1)} \sin^2(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}) = \frac{1}{\tau}[\frac{1}{2}\ln(1+\tau L)], \tag{A.0.38}$$

putting this value of integration back in A.0.29,

$$B^2 \frac{1}{\tau} \frac{\ln(1+\tau L)}{2} = 1, \tag{A.0.39}$$

with this, we can easily find the value of B,

$$B = \sqrt{\frac{2\tau}{\ln(1+\tau L)}}, \tag{A.0.40}$$

consequently by substituting the value of $m(x)^{\frac{1}{4}}$ and B in A.0.26,

$$\psi_n(x) = \frac{1}{(\tau x+a)^{\frac{1}{2}}} \sqrt{\frac{2\tau}{\ln(1+\tau L)}} \sin(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}), \tag{A.0.41}$$

as a=1, so

$$\psi_n(x) = \sqrt{\frac{2\tau}{(1+\tau x)\ln(1+\tau L)}} \sin(\frac{n\pi \ln(1+\tau x)}{\ln(1+\tau L)}). \tag{A.0.42}$$

Comparing A.0.12 and A.0.13 with the purpose to find the eigen energies of this position dependent effective mass system.

$$k^2 = 2E - \frac{\tau^2}{4}, \tag{A.0.43}$$

$$(\frac{n\pi\tau}{\ln(1+\tau L)})^2 = 2E_n - \frac{\tau^2}{4}, \tag{A.0.44}$$

$$\frac{n^2\pi^2\tau^2}{\ln^2(1+\tau L)} = 2E_n - \frac{\tau^2}{4}, \tag{A.0.45}$$

$$2E_n = \frac{\tau^2}{4} + \frac{n^2\pi^2\tau^2}{\ln^2(1+\tau L)}, \tag{A.0.46}$$

the eigen values,

$$E_n = \frac{\tau^2}{8} + \frac{n^2\pi^2\tau^2}{2\ln^2(1+\tau L)}. \tag{A.0.47}$$

Appendix B

Appendix

Increasing mass with position

$$m(x) = \frac{x^{\alpha}}{\tau^2}, \tag{B.0.1}$$

where $\alpha \neq -2$, by using the same transformation method, we can write

$$\psi(x) = m(x)^{\frac{1}{4}}\phi(y(x)) = \frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\phi(y(x)), \tag{B.0.2}$$

$$\frac{dy}{dx} = m(x)^{\frac{1}{2}} = \frac{x^{\frac{\alpha}{2}}}{\tau}, \tag{B.0.3}$$

Taking the derivative of ψ with respect to x,

$$\frac{d\psi}{dx} = \frac{\alpha}{4\tau^{\frac{1}{2}}}x^{\frac{\alpha}{4}-1}\phi(y(x)) + \frac{x^{\frac{3\alpha}{4}}}{\tau^{\frac{3}{2}}}\frac{d\phi}{dy}, \tag{B.0.4}$$

Schrödinger equation is

$$\frac{-1}{2}\frac{d}{dx}[\frac{1}{m(x)}\frac{d\psi}{dx}] + V(x)\psi(x) = E\psi(x), \tag{B.0.5}$$

putting the respective values in above equation from B.0.1 and B.0.4,

$$\frac{-1}{2}\frac{d}{dx}[\frac{\tau^2}{x^{\alpha}}(\frac{\alpha}{4\tau^{\frac{1}{2}}}x^{\frac{\alpha}{4}-1}\phi(y) + \frac{x^{\frac{3\alpha}{4}}}{\tau^{\frac{3}{2}}}\frac{d\phi}{dy})] = E\frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\phi(y(x)), \tag{B.0.6}$$

simplifying the equation,

$$\frac{-1}{2}\frac{d}{dx}[\frac{\alpha}{4}\frac{\tau^{\frac{3}{2}}}{x^{\frac{3\alpha}{4}+1}}\phi(y) + \frac{\tau^{\frac{1}{2}}}{x^{\frac{\alpha}{4}}}\frac{d\phi}{dy}] = E\frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\phi(y(x)), \tag{B.0.7}$$

again taking the derivative,

$$\frac{-1}{2}[-(\frac{3\alpha}{4}+1)\frac{\alpha}{4}\frac{\tau^{\frac{3}{2}}}{x^{\frac{3\alpha}{4}+2}}\phi(y)+\frac{\alpha}{4}\frac{\tau^{\frac{1}{2}}}{x^{\frac{\alpha}{4}+1}}\frac{d\phi}{dy}-\frac{\alpha}{4}\frac{\tau^{\frac{1}{2}}}{x^{\frac{\alpha}{4}+1}}\frac{d\phi}{dy}+\frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\frac{d^2\phi}{dy^2}]=E\frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\phi(y(x)), \tag{B.0.8}$$

simplifying the equation so that the first derivative terms vanish.

$$\frac{-1}{2}[(\frac{3\alpha+4}{4})\frac{\alpha}{4}\frac{\tau^{\frac{3}{2}}}{x^{\frac{3\alpha}{4}+2}}\phi(y)+\frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\frac{d^2\phi}{dy^2}]=E\frac{x^{\frac{\alpha}{4}}}{\tau^{\frac{1}{2}}}\phi(y(x)), \tag{B.0.9}$$

canceling $\frac{x^{\frac{\alpha}{4}}}{\tau^2}$ from both sides,

$$\frac{-1}{2}\frac{d^2\phi}{dy^2}+\frac{\alpha(3\alpha+4)}{8}\frac{1}{4x^(\alpha+2)}\phi(y)=E\phi(y), \tag{B.0.10}$$

from B.0.3, and let $\tau=1$,

$$\frac{dy}{dx}=x^{\frac{\alpha}{2}}, \tag{B.0.11}$$

$$\int dy=\int x^{\frac{\alpha}{2}}dx, \tag{B.0.12}$$

$$y=\frac{x^{\frac{\alpha}{2}+1}}{(\frac{\alpha}{2}+1)}, \tag{B.0.13}$$

then

$$x^{(\alpha+2)}=\frac{(\alpha+2)^2}{4}y^2, \tag{B.0.14}$$

$$\frac{-1}{2}\frac{d^2\phi}{dy^2}+\frac{\alpha(3\alpha+4)}{8(\alpha+2)^2y^2}\phi(y)=E\phi(y), \tag{B.0.15}$$

solution of this equation is,

$$\begin{aligned}\phi(y)=\sqrt{y(x)}BesselJ[\frac{(1+\alpha)}{2+\alpha},\sqrt{2E_n}y(x)]C[1]+\\ \sqrt{y(x)}BesselY[\frac{(1+\alpha)}{2+\alpha},\sqrt{2E_n}y(x)]C[2],\end{aligned} \tag{B.0.16}$$

$$\phi(y)=B_n\sqrt{y(x)}J_\beta(\sqrt{2E_n}y(x)). \tag{B.0.17}$$

where B_n is a normalization constant and $\beta=\frac{(1+\alpha)}{(2+\alpha)}$. Eigenvalues are given in zeros, z_n, of Bessel functions,

despite the fact we do not know about an exact expression of zeros, z_n, of Bessel function.

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