

Dynamical Behavior of The Morse Oscillator: The Coherent State Approach

by
Usama Zaheer



Supervised by
Dr. Shahid Iqbal

Submitted in the partial fulfillment of the

Degree of Master of Philosophy

In

Physics

School Of Natural Sciences,

National University of Sciences and Technology,

H-12, Islamabad, Pakistan.

*This Dissertation is dedicated
to my parents*

*for their endless love, support and
encouragement.*

Contents

1	Introduction	1
2	The Morse Oscillator	6
2.1	Introduction	6
2.2	Mathematical form of the Morse Oscillator Potential	7
2.3	Exact Solution to Schrödinger Equation	8
2.4	Limiting Behaviour Of Morse Potential	11
2.5	Applications in Different Fields	14
3	Coherent States in Quantum Mechanics	15
3.1	Introduction	15
3.2	Coherent States for Harmonic Oscillator and their Properties .	16
3.2.1	Algebraic Structure for Harmonic Oscillator	16
3.2.2	Construction	18
3.2.3	Properties of Coherent States	22
3.3	Generalized Coherent States	26
3.3.1	Barut-Giridello Coherent States	27
3.3.2	Perelomove Coherent States	28
3.3.3	Gazeau-Klauder (G.K) Coherent States	28
3.3.4	Gaussian Klauder Coherent States	30
4	The Coherent States for the Morse Oscillator	31
4.1	Introduction	31
4.2	Gazeau-Klauder Coherent States for Morse Oscillator	32
4.3	Statistical Measures of the Coherent State	33
4.4	Dynamical Behaviour of the Coherent State	35
4.4.1	Time Evolution of the Coherent State	35
4.4.2	Dynamics In Position Space	39
4.4.3	Dynamics in Momentum Space	43
4.4.4	The Phase Space Picture	47
4.4.5	Quasi Probability Distribution	50

5 Summary and Conclusion

List of Figures

2.1	Plots for different isotopes of Nitrogen molecules along with the corresponding values of ξ	8
2.2	Plots of the wavefunction $\psi_n(x)$ for different values of n	11
2.3	A graphical comparison between HO potential and MO potential	13
4.1	Dependence of $\langle n \rangle$ on the Model Parameter ζ in (a) $\zeta = 106$, $\langle n \rangle \approx 2$, (b) $\zeta = 251$, $\langle n \rangle \approx 5$, in (c) $\zeta = 451$, $\langle n \rangle \approx 10$ and in (d) $\zeta = 602$, $\langle n \rangle \approx 15$, also for numerics we have taken $\xi = 0.5$, $\vartheta \approx 0$, $\nu = 57.44$ and $n_{max} = 27$	34
4.2	Modulus square of auto correlation function (a) for $\langle n \rangle = 5$ and (b) for $\langle n \rangle = 10$	38
4.3	Probability distribution dependence on the coherent state parameter ζ at $t = 0$	40
4.4	Snap shots for probability density at different times.	41
4.5	Quantum carpet for one T_{qr} with $\zeta = 251$	42
4.6	Graphical comparison between the quantum carpet for coherent state of Morse oscillator and harmonic oscillator.	43
4.7	Probability density dependence on the coherent state parameter ζ at $t = 0$	44
4.8	Snap Shots of Probability density at Different Times.	45
4.9	Quantum Carpet for one T_{qr} with $\zeta = 251$	46
4.10	Graphical comparison between the quantum carpet for coherent state of Morse oscillator and Harmonic oscillator.	47
4.11	Expectation values for T_{qr} , $\tau = \frac{t}{T_{cl}}$	48
4.12	Plot for $\langle p \rangle$ for one T_{qr} with $\zeta = 251$, $\tau = \frac{t}{T_{cl}}$	49
4.13	phase space for one T_{qr} with $\zeta = 251$	50
4.14	Contour plot of wigner function for $\zeta = 251$	51
4.15	Contour plot of wigner function for $\zeta = 452$	52
4.16	Contour plot of wigner function for $\zeta = 602$	52

Acknowledgements

In the name of Allah who created this universe for us, to think and investigate His beauty.

I would like to dedicate my work firstly to my parents, for their endless prayers, love and support which really helped me to achieve this honourable degree from such a well reputed institution of Pakistan.

I would like to present my gratitude to my respected supervisor Dr. Shahid Iqbal for his kind supervision, support and motivation. His guidance helped me a lot during my research work. Whenever I was subjected to the difficulties his help proved worthy. He is a bit, strict but a kind hearted person and always showed affection to me. I will always remember his wonderful personality.

I specially want to thanks my guidance and examination committee members, Dr. Aeysha Khalique, Dr. Muddasir Ali Shah and Dr. Farhan Saif for their guidance and support for the improvement of my research work.

Lot of love, prayers, thanks to my friends Ahmad Ali (Scholar), Fahad Azad (Multanvi), Ali Adeel, Waqar Azeem (Discrete) for their beautiful memories. A very special thanks to Mr. Mureed Hussain Kamran Alvi in short (M.H.K.A) for his love, support and kindness I will never forget the Tea which I used to make for my friends and discussions during our Tea time. Lastly to a very special person Mr. Saqib Hussain Malik (Mussafir) a remarkable personality in my life, He told me what life exactly means.

I would also want to mention the duration I stayed in Rumi Hostels. It was a very beautiful period of my life, I have always enjoyed living in NUST

hostel. I always remember you my room 138 where I have written these lines.

I would also want to say thanks to my younger brothers Sohaib and Huzaifa and to my only sister Rida for their love and prayers. I feel my self very lucky to have you all in my life love you all.

Lastly I would extend my acknowledgements to the respected faculty members, staff and students of NUST-SNS for direct or indirect help.

Usama Zaheer

Abstract

The one-dimensional Morse oscillator in the context of generalized coherent states is discussed. It plays a vital role in the description of many physical oscillatory systems such as diatomic and polyatomic molecules. Using the Gazeau-Klauder formalism, the generalized coherent states for the Morse oscillator are constructed and their basic properties are discussed. The temporal characteristics of these states are analyzed by means of autocorrelation function and the phenomena of quantum revivals and fractional revivals are studied. Furthermore, we construct the time evolved coherent state wave packets both in position space and in momentum space to calculate the corresponding probability densities as a function of time. The time evolution of these probability densities result in the constructive and destructive interferences leading to the formation of quantum carpets. Moreover, we analyze the phase space properties by means of position-momentum expectation values and Wigner quasi probability distribution function. The negativity of the Wigner function reflects the nonclassicality of the constructed coherent states of the Morse oscillator.

Chapter 1

Introduction

The history of coherent states goes back to early days of modern quantum mechanics when Erwin Schrödinger was developing the wave mechanics. In 1926 he attempted to build quantum mechanical states manifesting dynamical behaviour close to classical dynamics. He succeeded to build quantum states for harmonic oscillator [1] and failed for general systems. In the context of wave mechanics, the centroids of the harmonic oscillator wave packets follow classical trajectories and minimise the uncertainty relation for the canonical variables involved. The expectation values of these canonical variables evolve in time in the same fashion as suggested by the classical theory for the harmonic oscillator.

The idea remained dormant for more than three decades before Roy Glauber in 1963 redefined these states [2–4] in terms of ladder operators of the harmonic oscillator. In a series of his seminal papers [2–4], he expressed the coherent electromagnetic field by means of these states, so they were named as coherent states. His ground breaking work laid the foundation of new field of quantum optics. He proposed three routes to define the coherent state as i) an eigen state of the annihilation operator; ii) a displaced ground state iii) a minimum uncertainty state. These three definitions were shown to be mutually equivalent. Later on these states were proved to be a cornerstone in many areas of physics and Glauber received the Nobel prize

in 2005 for his remarkable contribution.

The abundant applications of these states motivated the researchers to generalize the notion of coherent states. A generalized procedure for the construction of the coherent states for systems other than harmonic oscillator is required. The first mile stone in this regard was presented by Klauder in 1963 when he developed a generalized formalism to relate quantum dynamics with the classical dynamics [5]. In the same time Sudarshan described the semiclassical and quantum mechanical nature of light beams using their statistical behaviours [6]. In 1965 Klauder and McKenna jointly developed a generalized formalism for the diagonal representation of the coherent states using the density operators [7]. In their work they also discussed the Phase space representation for the coherent states. Later on Klauder and Sudarshan presented a description of the generalized coherent states based on Lie group algebra [8].

Most of the efforts to generalize the concept of coherent states were based on various algebraic groups. Klauder and Sudarshan presented the generalized coherent states based on Lie Group Algebra [8]. Barut and Girardello developed the coherent states for non compact groups [10], these states are known as Barut-Girardello coherent states. The concept was further generalized for all kind of lie groups by Perelomov [15] and the states are known as Perelomov coherent states. The work on generalized coherent states was beautifully collected and arranger by Klauder and Skagerstam in the form of a book [46]. In this work the literature was classified on the basis of the applications of the coherent states in different fields of physics and mathematics.

The available techniques to construct the generalized coherent states for various systems were explicitly based on the underlying algebra of the system. Therefore the available generalization techniques were not suitable to construct the coherent states for the systems whose algebraic structure was not known. It become necessary to develop some generalization techniques

for the construction of the coherent states which are independent of the algebraic structure of the system. In 1996 Klauder developed a formalism for the construction of coherent states of the system exhibiting discrete and degenerate energy spectra [11]. Later on the idea was extended by Gazeau and Klauder for general hamiltonian systems with bounded below non degenerate discrete and continuous energy spectrum. In this work a set of requirements was given, that should be satisfied by the states to be called as coherent states. This formalism attracted much attention of the researchers because of their algebraic independence. The coherent states were constructed based on the Gazeau-Klauder formalism for large variety of quantum mechanical systems such as pseudoharmonic oscillator [18], the Pöschl-Teller potential and the infinite square potential [19], the power law potentials [20,21], the triangular well potential [22] and the Morse oscillator potential [23,24]. In these articles various properties of the Gazeau-Klauder coherent states were studied for different hamiltonian systems. For example S. Iqbal. and F. Saif. in their work [20,21] have discussed the space time dynamics of Gazeau-Klauder coherent states for the power law potentials. In [22] they have studied the Gazeau-Klauder coherent states for Triangular well potential for which the underlying algebra does not exist and discussed its spatiotemporal characteristics. Another generalized approach for the construction of coherent states was introduced by R. Fox where he used a Gaussian function to approximate the behaviour of the coherent states. These Gaussian coherent states [13,14] are important because they efficiently resolve unity.

In present work we have focused on the construction of Gazeau-Klauder coherent states for the Morse oscillator potential. The Morse oscillator has a wide history starting from the work presented by P. M. Morse in 1929 [25], while solving the Schrödinger equation for the diatomic molecule. The Morse oscillator presents a realistic model for the vibrations of atoms in a diatomic or poly-atomic molecule, therefore it is equally important in the field of physics and chemistry. The Morse quantum system is one of the

quantum mechanical system which is exactly solvable and is based upon $SU(1,1)$ algebra.

Based upon its algebraic structure, the Barut-Girardello coherent states along with the harmonic limit were discussed for the Morse oscillator [16]. Sánchez and Récamier used the f -deformed oscillator formalism (basically an algebra dependent formalism) to discuss the squeezed coherent states for Morse oscillator along with the phase space representation and corresponding Wigner function [17]. An excellent collection of work done so far on the Morse oscillator was published by Dong in the year 2007 [26]. In this book exact solution, ladder operators, matrix elements, harmonic limit, Franck-Condon factor, transition probabilities and associate Lie algebra was discussed for the Morse oscillator. Generalized coherent states for the Morse oscillator were discussed by Angelova and Hussin. They studied the squeezed coherent states for Morse quantum system and analysed its various properties like localization in position space and minimization of Heisenberg uncertainty relation. They also have given a phase space picture for a short time interval [31,32]. Based on this work, we will try to develop Gazeau-Klauder coherent states for the Morse oscillator and present a complete dynamical picture for these states both in position and momentum space.

Our work is organized as follows. In Chapter 2 we discuss the Morse oscillator, reduction to harmonic oscillator (harmonic limit), exact solution for the corresponding Schrödinger equation and its uses in different fields. Chapter 3 is dedicated to the generalized coherent states, here we will derive the coherent state for harmonic oscillator using Glauber's definitions and discuss its various properties. Then we will discuss the various generalization introduced for the construction of coherent states for the general hamiltonian systems. Chapter 4 is dedicated to the construction of generalized Gazeau-klauder coherent states for the Morse potential, its revival dynamics in position as well as momentum space, its phase space representation using the expectation values in position and momentum space and

the Wigner quasi probability distribution function. We conclude our work in Chapter 5.

Chapter 2

The Morse Oscillator

2.1 Introduction

In 1929 P.M. Morse introduced the Morse Potential [25] while finding an exact solution for the Schrödinger equation which represents the realistic model for the oscillations of the nuclei in a diatomic molecule. This potential has diverse uses in the fields of Physics and Chemistry which we will discuss at the end of this chapter. So far among the known quantum physical systems, very few of them are exactly solvable for example harmonic oscillator and hydrogen atom. Before 1929 harmonic oscillator potential was used to model the oscillations of nuclei in a diatomic molecule. The harmonic oscillator potential does not account for the an-harmonic behaviour of the diatomic or poly-atomic molecules. But after the introduction of Morse potential it takes the place of harmonic oscillator potential. This is because Morse potential efficiently accounts for the an-harmonic behaviour of the diatomic or poly-atomic molecules. In literature we can find two main equivalent ways to find the eigen values and eigen function for the Morse potential. The first method is relatively a difficult approach by Landau and Lifshitz [27] but it is remarkable. In this method the underlying algebra was developed for the Morse potential using SUSYQM method and ladder operators were developed. Second method at which we have focused in our research work

is by solving the corresponding Schrödinger wave equation as proposed by P.M. Morse.

This chapter is dedicated to the Morse oscillator. In section 2.2 we discuss the mathematical form of the Morse potential. In section 2.3 we present an exact solution to the Schrödinger equation for Morse oscillator. In section 2.4 we try to reduce our Morse potential into harmonic oscillator potential under the harmonic limit and will give a graphical comparison between the both potentials. Section 2.5 is dedicated to some of the uses of this potential in different fields.

2.2 Mathematical form of the Morse Oscillator Potential

The generalized mathematical form of the Morse potential [25] that was proposed by P. M. Morse is

$$V(x) = V_0 e^{-2\xi(x-x_0)} - 2V_0 e^{-\xi(x-x_0)}, \quad (2.2.1)$$

where $V_0 = \frac{\omega_e^2}{4\omega_e x_e}$ is the potential energy at equilibrium position and related to the depth of potential at equilibrium, ω_e is the vibrational constant, $\omega_e x_e$ is the anharmonicity constant, ξ is the parameter of the model related to the depth and width of the potential and is dependent upon the anharmonicity constant by the relation $\xi = 0.2454(\sqrt{\mu\omega_e x_e})$, x_0 is the distance between the diatomic molecule at the equilibrium and x represents the displacement from the equilibrium position. These above mentioned constants are called the spectroscopic constants [29]. We have used the values of these spectroscopic constants for different isotopes of Nitrogen molecule in figure 2.1 where each colour represents a different isotope.

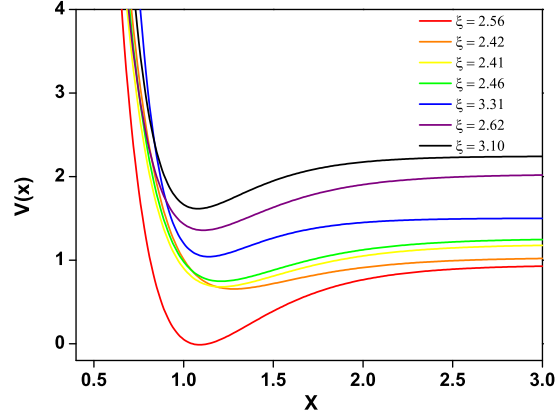


Figure 2.1: Plots for different isotopes of Nitrogen molecules along with the corresponding values of ξ

2.3 Exact Solution to Schrödinger Equation

The Morse quantum system is exactly solvable [26] and this section provides us a complete description of the solution. The one dimensional Schrödinger wave equation can be written as

$$\left(\frac{-\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) \right) \psi(x) = E\psi(x), \quad (2.3.1)$$

where μ is the reduced mass of the system and we have taken the Morse potential given in eq. (2.2.1) in simplified form in one dimension as

$$V(x) = V_0 \left(e^{-2\xi x} - 2e^{-\xi x} \right), \quad (2.3.2)$$

where V_0 is the potential at the mean position, ξ is the parameter of the system related to depth and width of the potential and x represents the displacement. Using eq. (2.3.2) in eq. (2.3.1) we get

$$\left(\frac{-\hbar^2}{2\mu} \frac{d^2}{dx^2} + V_0 \left(e^{-2\xi x} - 2e^{-\xi x} \right) \right) \psi(x) = E\psi(x), \quad (2.3.3)$$

which on rearranging becomes

$$\frac{d^2}{dx^2} \psi(x) + \frac{2\mu}{\hbar^2} \left(E - V_0 e^{-2\xi x} + 2V_0 e^{-\xi x} \right) \psi(x) = 0. \quad (2.3.4)$$

Let us introduce the following substitutions $y = \frac{2\sqrt{2\mu V_0}}{\xi\hbar} e^{-\xi x}$, The derivative of y with respect to x can be written as $\frac{dy}{dx} = \frac{-2\sqrt{2\mu V_0}}{\hbar} e^{-\xi x}$ which simply equals to $\frac{dy}{dx} = \xi y$. Now the derivative of $\Psi(x)$ with respect to x can be written as $\frac{d\psi(x)}{dx} = \frac{d\psi(y)}{dy} \frac{dy}{dx}$ by chain rule and can be further simplified as $\frac{d\psi(x)}{dx} = \frac{d\psi(y)}{dy} \xi y$. The second derivative of $\psi(x)$ is $\frac{d^2\psi(x)}{dx^2} = \frac{d}{dx} \left(\frac{d\psi(y)}{dy} \right) \xi y = \frac{d}{dy} \left(\frac{d\psi(y)}{dy} \frac{dy}{dx} \right) \xi y$, which on performing derivative can be written as $\frac{d^2\psi(x)}{dx^2} = \left(\frac{d^2\psi(y)}{dy^2} \xi y + \frac{d\psi(y)}{dy} \xi \right) \xi y$. This can simply be written as

$$\frac{d^2\psi(x)}{dx^2} = \psi''(y)\xi^2 y^2 + \psi'(y)\xi^2 y. \quad (2.3.5)$$

Also

$$e^{-\xi x} = \frac{\xi\hbar y}{2\sqrt{2\mu V_0}}, \quad (2.3.6)$$

$$e^{-2\xi x} = \frac{\xi^2 \hbar^2 y^2}{8\mu V_0}. \quad (2.3.7)$$

Using eq. (2.3.5), eq. (2.3.6) and eq. (2.3.7) in eq. (2.3.4) we get

$$\psi''(y)\xi^2 y^2 + \psi'(y)\xi^2 y + \frac{2\mu}{\hbar^2} \left(E - V_0 \frac{\xi^2 \hbar^2 y^2}{8\mu V_0} + 2V_0 \frac{\xi\hbar y}{2\sqrt{2\mu V_0}} \right) \psi(y) = 0. \quad (2.3.8)$$

On simplification eq. (2.3.8) becomes

$$\psi''(y) + \frac{\psi'(y)}{y} + \frac{2\mu E}{\xi^2 \hbar^2 y^2} \psi(y) - \frac{1}{4} \psi(y) + \frac{\sqrt{2\mu V_0}}{\xi\hbar y} \psi(y). \quad (2.3.9)$$

Now in order to define our wavefunction $\psi(y)$ in the limits from 0 to ∞ , we make some more substitutions by introducing the following variables

$$s = \frac{\sqrt{-2\mu E}}{\xi\hbar}, \quad (2.3.10)$$

$$n = \frac{\sqrt{2\mu V_0}}{\xi\hbar} - \left(s + \frac{1}{2} \right). \quad (2.3.11)$$

Using eq. (2.3.10), eq. (2.3.11) in eq. (2.3.9) we get

$$\psi''(y) + \frac{\psi'(y)}{y} + \left(-\frac{1}{4} + \frac{1}{y} \left(n + s + \frac{1}{2} \right) \right) \psi(y) = 0. \quad (2.3.12)$$

Our wavefunction must be finite and it must behave as $e^{-\frac{y}{2}}$ at $y \rightarrow \infty$ and as y^s if $y \rightarrow 0$, so we may write our wavefunction as

$$\psi(y) = e^{-\frac{y}{2}} y^s w(y), \quad (2.3.13)$$

where $w(y)$ is an unknown function of y . In order to find it we may take first and second derivatives of eq. (2.3.13) i.e $\psi'(y)$ and $\psi''(y)$ and substituting their values in eq. 2.3.12 we get a second order differential equation for $w(y)$ which can be written as

$$yw''(y) + (2s + 1 - y)w'(y) + nw(y) = 0. \quad (2.3.14)$$

The above equation is an equation for a confluent hypergeometric function. We need to find the solution of this equation under the conditions that when $y \rightarrow 0$, $w(y)$ is finite and when $y \rightarrow \infty$, $w(y)$ tends to infinity not more rapidly than every finite power of y . These conditions can be satisfied by considering the $F(-n, 2s + 1, y)$ form of confluent hypergeometric function which may reduced to a polynomial called Associated Laguerre polynomials given as

$$L_n^{2s+1}(y) = (-1)^{2s+1} \frac{n!}{(n - 2s + 1)!} e^y y^{-2s-1} \frac{d^{n-2s-1}}{dy^{n-2s-1}} \left(e^{-y} (2s+1)^n \right). \quad (2.3.15)$$

We may ignore 1 form $2s + 1$ and can take it as $2s$

$$L_n^{2s}(y) = (-1)^{2s} \frac{n!}{(n - 2s)!} e^y y^{-2s} \frac{d^{n-2s}}{dy^{n-2s}} \left(e^{-y} (2s)^n \right). \quad (2.3.16)$$

Hence we see that the unknown function $w(y)$ is $L_n^{2s}(y)$ and therefore our wavefunction $\Psi(y)$ can be written as we may also convert the variable y into x for our the ease of discussion in further calculations.

$$\psi_n(x) = N_n e^{-\frac{x}{s}} x^s L_n^{2s}(x), \quad (2.3.17)$$

where, N_n is the normalization constant and is given as

$$N_n = \sqrt{\frac{\xi(\nu - 2n - 1)\Gamma(n + 1)}{\Gamma(\nu - n)}}, \quad (2.3.18)$$

where ν is defined as $\nu = \sqrt{\frac{8\mu V_0}{\xi^2 \hbar^2}}$ and provides the truncation of energy spectrum which can be written using eq. (2.3.10) as

$$E_n = -\frac{\hbar^2}{2\mu} s^2 \xi^2, \quad (2.3.19)$$

and $s = \frac{\nu-1}{2} - n$ which also shows that n can take only discrete but finite values and the maximum number of values which n can take is given by $\frac{\nu-1}{2}$. Here we also want to show the plots for the wavefunction $\psi_n(x)$ for different values of n as in Figure 2.2.

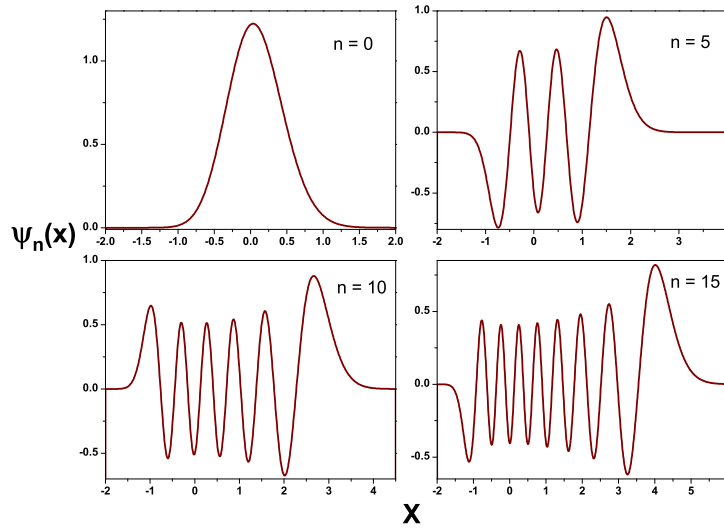


Figure 2.2: Plots of the wavefunction $\psi_n(x)$ for different values of n

2.4 Limiting Behaviour Of Morse Potential

As the scientific society always took interest in the simplification of the complicated system into a simple system. Therefore here we are going to have a look on the simplification of our potential given by eq. (2.2.1). We have already discussed that before the introduction of morse potential harmonic oscillator potential was used to model the vibrations of the diatomic molecules

and other related situations. The atomic vibration of these diatomic or polyatomic molecules are not harmonic in nature. The best suited model is that which is presented by Morse in the form of Morse potential eq. (2.2.1), which accounts well for the anharmonicity of the molecules. Now the question is: Is there any limit under which this Morse potential can be reducible to the harmonic oscillator potential? The answer is, yes we can reduce The Morse potential to the harmonic oscillator potential. Actually the anharmonicity in the vibrations of the molecules arises as a result of increasing vibrational amplitudes. Near equilibrium there is least anharmonicity and our system behaves harmonically. This restriction to study the system near equilibrium is called the "*Harmonic Limit for Morse oscillator potential*". Let us elaborate the procedure as suggested by Popov in [30]. The Morse potential as given in eq. (2.2.1) can also be written as

$$V(x) = V_0 \left(1 - e^{-\xi x} \right)^2. \quad (2.4.1)$$

Imposing the limit that near equilibrium the product of $\xi x \rightarrow 0$ such that in the series expansion of the involving exponential function eq. (2.4.1) its square and higher powers can be neglected. that is

$$V(x) = V_0 \left(1 - (1 - \xi x) \right)^2, \quad (2.4.2)$$

which on further simplification gives

$$V(x) = V_0 \xi^2 x^2. \quad (2.4.3)$$

Comparison of above equation and the harmonic oscillator potential $V_{HO} = \frac{m\omega^2 x^2}{2}$ leads us to the relation between the spectroscopic constants discussed above and the mass m and frequency ω as $\frac{m\omega^2}{2} = V_0 \xi^2$. This relation has the units of the spring constant k i.e (Kg/s^2). We can also show a comparison between the harmonic oscillator potential (HO) and the Morse oscillator potential (MO) by Figure 2.3.

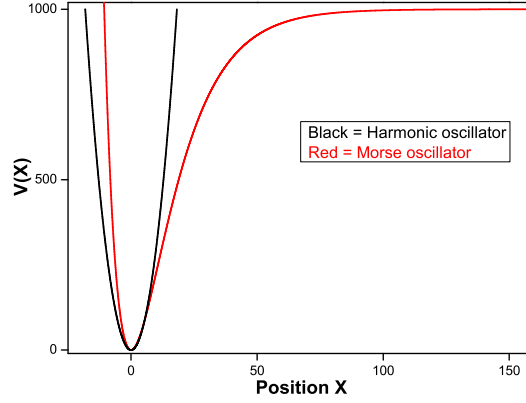


Figure 2.3: A graphical comparison between HO potential and MO potential

The energy spectrum given by eq. (2.3.19) for morse oscillator, can also be reduced to the harmonic oscillator energy spectrum under harmonic limit by using the following relation,

$$\frac{m\omega^2}{2} = V_0\xi^2, \quad (2.4.4)$$

which we already discussed above. The eq. (2.3.19) reads as

$$E_n = -\frac{\hbar^2}{2\mu} s^2 \xi^2, \quad (2.4.5)$$

with,

$$s = \frac{\nu - 1}{2} - n, \quad \nu = \sqrt{\frac{8\mu V_0}{\xi^2 \hbar^2}}. \quad (2.4.6)$$

Using the values s and ν in eq. (2.4.5) we get

$$E_n = -V_0 + \hbar\xi \sqrt{\frac{2V_0}{\mu}} \left(n + \frac{1}{2}\right) - \frac{\hbar^2 \xi^2}{2\mu} \left(n + \frac{1}{2}\right)^2. \quad (2.4.7)$$

By using the relation given by eq. (2.4.4) above equation becomes

$$E_n = -V_0 + \hbar\omega \left(n + \frac{1}{2}\right) - \frac{\hbar^2 \omega^2}{4V_0} \left(n + \frac{1}{2}\right)^2, \quad (2.4.8)$$

which is just another way to write eq. (2.3.19). According to the harmonic limit $\xi \rightarrow 0$ such that its square and higher values can be neglected, using this condition eq. (2.4.7) get reduced to

$$E_n \equiv \hbar\xi \sqrt{\frac{2V_0}{\mu}} \left(n + \frac{1}{2} \right) = \hbar\omega \left(n + \frac{1}{2} \right), \quad (2.4.9)$$

which is the energy spectrum for harmonic oscillator.

2.5 Applications in Different Fields

The Morse potential has wide range of application in different fields of physics and chemistry. The Morse potential was used in the field of quantum optics where its generalized and gaussian coherent states were studied using the underlying algebra by Angelova and Hussin [31, 32]. The work done by Jarman and Fraser [33] for the calculation of transition probabilities is remarkable. Having the transition probabilities in hand we can easily calculate the matrix elements numerically [34–36]. In literature, people use this potential in various calculations like variational method to investigate equilibrium thermodynamic behaviour of quantum morse chain[37], phase shift to the partition function was presented for a diatomic molecule model [38], on the calculation of the wigner distribution function [39–41]. Also some of the applications of morse potential can also be found in the field of solid state physics related to the physical properties of the materials including all the spectroscopic constants [29] and it also includes the study of binding energies, stabilities of different kind of materials, the point defect, the line defect etc.

Chapter 3

Coherent States in Quantum Mechanics

3.1 Introduction

In 1926, Schrödinger introduced coherent states as some superposition of energy eigenstates of quantum harmonic oscillator [1] whose dynamics is closely related to the behaviour of the classical harmonic oscillator and most importantly these states minimize the uncertainty relation. After Schrödinger this idea did not flourish for almost 2 decades. In 1963 Glauber [2–4] extended the idea working in context of quantum aspects of light. He showed that electromagnetic field states have classical behaviour and named them as coherent states. As harmonic oscillator is of fundamental importance in quantum mechanics. It not only help us to understand the basic ideas of quantum mechanics, rather it also have much practical applications. As we have discussed in the previous chapter that Morse oscillator can be reduced to harmonic oscillator under harmonic limit. Therefore it is quite reasonable at this stage to first discuss the coherent states for harmonic oscillator and than we look for the generalizations to the other hamiltonian systems.

This chapter contains a review on the coherent states of the harmonic oscillator in section 3.2 including the properties satisfied by these states. The section 3.3 is dedicated to the generalized coherent states in which we

will briefly discuss the different types of coherent states that can be found in literature and will try to provide some details about the Gazeau-Klauder coherent states with some of its uses.

3.2 Coherent States for Harmonic Oscillator and their Properties

3.2.1 Algebraic Structure for Harmonic Oscillator

The hamiltonian \hat{H} for harmonic oscillator can be written using the two canonical operators \hat{x} for position and \hat{p} for momentum as

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + \frac{\mu\omega^2\hat{x}^2}{2}, \quad (3.2.1)$$

where \hat{x} and \hat{p} are Hermitian and ω is the frequency of the oscillator related to spring constant k as $\omega = \sqrt{\frac{k}{\mu}}$. Let us here define two non-Hermitian operators

$$\hat{a} = \sqrt{\frac{\mu\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{\mu\omega} \right), \quad \hat{a}^\dagger = \sqrt{\frac{\mu\omega}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{\mu\omega} \right), \quad (3.2.2)$$

these operators are named as annihilation and creation operators, the reason for their naming will be explained shortly. Their commutation relation is

$$[\hat{a}, \hat{a}^\dagger] = 1. \quad (3.2.3)$$

Also we define a number operator as

$$\hat{N} = \hat{a}^\dagger \hat{a}, \quad (3.2.4)$$

which is a Hermitian operator. We can write our hamiltonian \hat{H} in terms of this number operator as

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right). \quad (3.2.5)$$

Now as \hat{H} can be written in terms of \hat{N} , therefore they can have simultaneous eigenkets. We can represent the action of the number operator on the energy eigenket $|n\rangle$ as

$$\hat{N}|n\rangle = n|n\rangle, \quad (3.2.6)$$

where n is the corresponding eigenvalue. This n can have only nonnegative values, as

$$\hat{H}|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle, \quad (3.2.7)$$

which means that the corresponding energy eigenvalues are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \quad (3.2.8)$$

Now if n can take negative values the energy becomes negative, which is not possible. The ground state energy for harmonic oscillator is $E_0 = \frac{1}{2}\hbar\omega$.

Now we are going to explain the reason for naming \hat{a} as annihilation operator and \hat{a}^\dagger as creation operator. Let us note the following commutation relations

$$[\hat{N}, \hat{a}] = -\hat{a}, \quad [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger. \quad (3.2.9)$$

If we study the operation of \hat{N} on the state $\hat{a}^\dagger|n\rangle$ using eq. 3.2.9, we get the resultant eigenvalue increased by one as

$$\hat{N}\hat{a}^\dagger|n\rangle = (n+1)\hat{a}^\dagger|n\rangle. \quad (3.2.10)$$

Similarly the operation of \hat{N} on the state $\hat{a}|n\rangle$, we get the resultant eigenvalue decreased by one as

$$\hat{N}\hat{a}|n\rangle = (n-1)\hat{a}|n\rangle. \quad (3.2.11)$$

Using eq. (3.2.10) and eq. (3.2.11) we get

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (3.2.12)$$

Hence the above equation explain the reason for naming \hat{a} as annihilation operator as it annihilate the number state to one level similarly the creation operator \hat{a}^\dagger adds one level to the number state. From last result of eq. (3.2.12), we may observe that we can obtain state $|n\rangle$ by the successive action of creation operator \hat{a}^\dagger on the vacuum state $|0\rangle$ i.e,

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (3.2.13)$$

As \hat{H} and \hat{N} are Hermitian operators and $|n\rangle$ are simultaneous eigenstates of these operators, therefore number states $|n\rangle$ are orthogonal i.e $\langle n'|n\rangle = \delta_{nn'}$. In addition these states forms complete basis and their completeness relation is given as

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = 1. \quad (3.2.14)$$

3.2.2 Construction

Glauber proposed three equivalent definitions for the coherent states. Let us see the construction of the coherent states of harmonic oscillator using these definitions.

As an Eigenstate of the Annihilation Operator

The harmonic oscillator annihilation operator \hat{a} is given by eq. (3.2.2), using this operator we can define coherent state $|\alpha\rangle$ as

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \quad (3.2.15)$$

where α is complex entity. In order to derive an explicit expression for our coherent state $|\alpha\rangle$, we need to expand our coherent state in terms of eigenstates of the number operator $|n\rangle$. We can perform this expansion by writing $|\alpha\rangle$ as

$$|\alpha\rangle = \sum_{n=0}^{\infty} |n\rangle\langle n|\alpha\rangle, \quad (3.2.16)$$

where we have used the completeness relation of number state given by eq. (3.2.14). Now $\langle n|\alpha\rangle$ can be determined by projecting $\langle n|$ on eq. (3.2.15),

$$\langle n|\hat{a}|\alpha\rangle = \alpha\langle n|\alpha\rangle. \quad (3.2.17)$$

The complex conjugation of the relation $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ given by eq. (3.2.12), is $\langle n|\hat{a} = \sqrt{n+1}\langle n+1|$. Using this result in eq. (3.2.17) we get

$$\sqrt{n+1}\langle n+1|\alpha\rangle = \alpha\langle n|\alpha\rangle. \quad (3.2.18)$$

Replacing $n + 1$ by n , we have $\sqrt{n}\langle n|\alpha\rangle = \alpha\langle n - 1|\alpha\rangle$ we can write

$$\langle n|\alpha\rangle = \frac{\alpha}{\sqrt{n}}\langle n - 1|\alpha\rangle. \quad (3.2.19)$$

In addition $\langle n - 1|\alpha\rangle = \frac{\alpha}{\sqrt{n-1}}\langle n - 2|\alpha\rangle$ and hence

$$\langle n|\alpha\rangle = \frac{\alpha^2}{\sqrt{n}\sqrt{n-1}}\langle n - 2|\alpha\rangle. \quad (3.2.20)$$

If we repeat the above step n times we eventually get

$$\langle n|\alpha\rangle = \frac{\alpha^n}{\sqrt{n!}}\langle 0|\alpha\rangle. \quad (3.2.21)$$

Using above relation in eq. (3.2.16) we have

$$|\alpha\rangle = \langle 0|\alpha\rangle \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle, \quad (3.2.22)$$

where $\langle 0|\alpha\rangle$ is a constant and can be found by normalization of above equation i.e $\langle \alpha|\alpha\rangle = 1$

$$\langle \alpha|\alpha\rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \frac{\alpha^{*m}}{\sqrt{m!}} |\langle 0|\alpha\rangle|^2 \langle m|n\rangle. \quad (3.2.23)$$

At $m = n$ above equation becomes $1 = |\langle 0|\alpha\rangle|^2 \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!}$ which will give

$$\langle 0|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}. \quad (3.2.24)$$

Using eq. (3.2.24) in eq. (3.2.22) we can get the required expansion of $|\alpha\rangle$ in terms of the eigenstates of number operator as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \quad (3.2.25)$$

The above equation provides us an explicit expression for the coherent state of harmonic oscillator.

As Displaced Vacuum States

The second definition implies that the coherent states can be obtained by operating the displacement operator $\hat{D}(\alpha)$ on to the vacuum state of harmonic oscillator. This displacement operator [9] can be written in terms of annihilation and creation operator of harmonic oscillator and is defined as.

$$\hat{D}(\alpha) = e^{(\alpha\hat{a}^\dagger - \alpha^*\hat{a})}. \quad (3.2.26)$$

Therefore using $\hat{D}(\alpha)$ the coherent state can be written by definition as

$$|\alpha\rangle = \hat{D}(\alpha)|0\rangle. \quad (3.2.27)$$

Now here we consider the famous Baker-Hausdorff identity which reads as

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]} = e^{\hat{B}}e^{\hat{A}}e^{\frac{1}{2}[\hat{A},\hat{B}]}. \quad (3.2.28)$$

This identity is valid only if $[\hat{A}, \hat{B}] \neq 0$ and $[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$.

By taking $\hat{A} = \alpha\hat{a}^\dagger$ and $\hat{B} = -\alpha^*\hat{a}$ and $[\hat{A}, \hat{B}] = |\alpha|^2$ we can write eq. (3.2.26) as

$$\hat{D}(\alpha) = e^{-\frac{1}{2}|\alpha|^2}e^{\alpha\hat{a}^\dagger}e^{\alpha^*\hat{a}}. \quad (3.2.29)$$

By taking series expansion of $e^{\alpha^*\hat{a}}$ where \hat{a} is the annihilation operator, its action on $|0\rangle$ i.e ground state gives

$$e^{\alpha^*\hat{a}}|0\rangle = \sum_{l=0}^{\infty} \frac{(-\alpha^*)^l}{l!}(\hat{a})^l|0\rangle. \quad (3.2.30)$$

As $(\hat{a})^l|0\rangle = 0$ except only when $l = 0$ the above equation gives

$$e^{\alpha^*\hat{a}}|0\rangle = 0. \quad (3.2.31)$$

By taking the series expansion of $e^{\alpha\hat{a}^\dagger}$ where \hat{a}^\dagger is the creation operator, its action on the ground state $|0\rangle$ gives

$$e^{\alpha\hat{a}^\dagger}|0\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}(\hat{a}^\dagger)^n|0\rangle. \quad (3.2.32)$$

As $(\hat{a}^\dagger)^n|0\rangle = \sqrt{n!}|n\rangle$ the above equation gives

$$e^{\alpha\hat{a}^\dagger}|0\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \quad (3.2.33)$$

Now by using eq. (3.2.29) along with eq. (3.2.31) and eq. (3.2.33) in eq. (3.2.27) we get our coherent state as

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \quad (3.2.34)$$

As Minimum Uncertainty States

Both Glauber and Schrödinger agree with this definition that the coherent states of harmonic oscillator minimizes the uncertainty relation for the involved canonical variables. For harmonic oscillator, the dimensionless canonical position and momentum operators can be defined as

$$\hat{X} = \frac{1}{2}(\hat{a} + \hat{a}^\dagger), \quad (3.2.35)$$

$$\hat{P} = \frac{1}{2i}(\hat{a} - \hat{a}^\dagger). \quad (3.2.36)$$

We are now interested in finding out the dispersions in these quadratures with respect to our coherent state $|\alpha\rangle$ using the formulas

$$\Delta x = \sqrt{\langle\hat{X}^2\rangle_\alpha - \langle\hat{X}\rangle_\alpha^2}, \quad (3.2.37)$$

$$\Delta p = \sqrt{\langle\hat{P}^2\rangle_\alpha - \langle\hat{P}\rangle_\alpha^2}. \quad (3.2.38)$$

Now we calculate $\langle\hat{X}^2\rangle_\alpha$, $\langle\hat{X}\rangle_\alpha$, $\langle\hat{P}^2\rangle_\alpha$ and $\langle\hat{P}\rangle_\alpha$. and make use of these identities $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$, $\langle\alpha|\hat{a}^\dagger = \alpha^*\langle\alpha|$

$$\langle\hat{X}\rangle_\alpha = \frac{1}{2}\langle\alpha|(\hat{a} + \hat{a}^\dagger)|\alpha\rangle, \quad (3.2.39)$$

Which by using above identities and $\langle\alpha|\alpha\rangle$ becomes

$$\langle\hat{X}\rangle_\alpha = \frac{1}{2}[\alpha + \alpha^*]. \quad (3.2.40)$$

In addition $\langle \hat{X}^2 \rangle_\alpha$ can be calculated as follows

$$\langle \hat{X}^2 \rangle_\alpha = \langle \alpha | \hat{X} \hat{X} | \alpha \rangle, \quad (3.2.41)$$

$$\langle \hat{X}^2 \rangle_\alpha = \frac{1}{4} \langle \alpha | (\hat{a} + \hat{a}^\dagger)(\hat{a} + \hat{a}^\dagger) | \alpha \rangle, \quad (3.2.42)$$

which on using the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$ and performing simplification becomes

$$\langle \hat{X}^2 \rangle_\alpha = \frac{1}{4} \langle \alpha | \hat{a} \hat{a} + 2\hat{a}^\dagger \hat{a} + \hat{a}^\dagger \hat{a}^\dagger + 1 | \alpha \rangle. \quad (3.2.43)$$

Using the above identities above equation takes the form

$$\langle \hat{X}^2 \rangle_\alpha = \frac{1}{4} (\alpha^2 + 2\alpha^* \alpha + \alpha^{*2} + 1), \quad (3.2.44)$$

$$\langle \hat{X}^2 \rangle_\alpha = \frac{1}{4} ((\alpha + \alpha^*)^2 + 1). \quad (3.2.45)$$

Similarly we can calculate $\langle \hat{P} \rangle_\alpha$, $\langle \hat{P}^2 \rangle_\alpha$ and they have the forms

$$\langle \hat{P} \rangle_\alpha = \frac{1}{2i} [\alpha - \alpha^*], \quad (3.2.46)$$

$$\langle \hat{P}^2 \rangle_\alpha = -\frac{1}{4} ((\alpha - \alpha^*)^2 - 1). \quad (3.2.47)$$

By using eq. (3.2.40), eq. (3.2.45) in eq. (3.2.37) we get

$$\Delta x = \sqrt{\frac{1}{4} ((\alpha + \alpha^*)^2 + 1) - \frac{1}{4} (\alpha + \alpha^*)^2} = \frac{1}{2}, \quad (3.2.48)$$

Similarly, by using eq. (3.2.46), eq. (3.2.47) in eq. (3.2.38) we get

$$\Delta p = \sqrt{-\frac{1}{4} ((\alpha - \alpha^*)^2 + 1) + \frac{1}{4} (\alpha - \alpha^*)^2} = \frac{1}{2}. \quad (3.2.49)$$

Hence $\Delta x \Delta p = \frac{1}{4}$ which is the minimum uncertainty condition for harmonic oscillator. Therefore harmonic oscillator coherent state $|\alpha\rangle$ are the minimum uncertainty states with equal uncertainty in each quadrature.

3.2.3 Properties of Coherent States

Now in this section we will discuss some of the properties of the coherent states. These states satisfy a special set of properties which are

Orthogonality

A coherent state say $|\alpha\rangle$ is orthogonal to a state $|\beta\rangle$ if $\langle\beta|\alpha\rangle = 0$. In order to prove this we study the overlap of two different coherent states of harmonic oscillator say $|\alpha\rangle, |\beta\rangle$ generated by the action of there corresponding displacement operators $\hat{D}(\alpha)$ and $\hat{D}(\beta)$ on the vacuum state as $|\alpha\rangle = \hat{D}(\alpha)|0\rangle$, $|\beta\rangle = \hat{D}(\beta)|0\rangle$. We are now interested in the overlap $\langle\beta|\alpha\rangle$ i.e

$$\langle\beta|\alpha\rangle = \langle 0|\hat{D}^\dagger(\beta)\hat{D}(\alpha)|0\rangle. \quad (3.2.50)$$

Where $\hat{D}(\alpha) = e^{-\frac{1}{2}|\alpha|^2}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}$ and $\hat{D}^\dagger(\beta) = e^{-\frac{1}{2}|\beta|^2}e^{-\beta\hat{a}^\dagger}e^{\beta^*\hat{a}}$. Using these in above equation we get

$$\langle\beta|\alpha\rangle = \langle 0|\left(e^{-\frac{1}{2}|\beta|^2}e^{-\beta\hat{a}^\dagger}e^{\beta^*\hat{a}}\right)\left(e^{-\frac{1}{2}|\alpha|^2}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}\right)|0\rangle. \quad (3.2.51)$$

Above equation can also be written as

$$\langle\beta|\alpha\rangle = e^{-\frac{1}{2}(|\beta|^2+|\alpha|^2)}\langle 0|e^{-\beta\hat{a}^\dagger}e^{\beta^*\hat{a}}e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}|0\rangle. \quad (3.2.52)$$

By applying Taylor series expansion to the outer two operators i.e $e^{-\beta\hat{a}^\dagger} = \left(1 - (\beta\hat{a}^\dagger) + \dots\right)$ and $e^{-\alpha^*\hat{a}} = \left(1 - (\alpha^*\hat{a}) + \dots\right)$. Operating these expression onto the left and right respectively using $\langle 0|\hat{a}^\dagger = 0$ and $\hat{a}|0\rangle = 0$, the higher order terms vanishes and the eq. (3.2.52) reduces to

$$\langle\beta|\alpha\rangle = e^{-\frac{1}{2}(|\beta|^2+|\alpha|^2)}\langle 0|e^{\beta^*\hat{a}}e^{\alpha\hat{a}^\dagger}|0\rangle. \quad (3.2.53)$$

Again by taking the Taylor expansion of the involved exponentials i.e $e^{\beta^*\hat{a}} = \left(1 + (\beta^*\hat{a}) + \frac{(\beta^*\hat{a})^2}{2!} + \dots\right)$ and $e^{\alpha\hat{a}^\dagger} = \left(1 + (\alpha\hat{a}^\dagger) + \frac{(\alpha\hat{a}^\dagger)^2}{2!} + \dots\right)$ the eq. (3.2.53) takes the form

$$\langle\beta|\alpha\rangle = \left(\langle 0| + \beta^*\langle 1| + \frac{\beta^{*2}\sqrt{2}}{2!}\langle 2| + \dots\right)\left(|0\rangle + \alpha|1\rangle + \frac{\alpha^2\sqrt{2}}{2!}|2\rangle + \dots\right)e^{-\frac{1}{2}(|\beta|^2+|\alpha|^2)}, \quad (3.2.54)$$

Using orthogonality of the number state, the above equation reduces to

$$\langle\beta|\alpha\rangle = \left(1 + \alpha\beta^* + \frac{(\alpha\beta^*)^2}{2!} + \dots\right)e^{-\frac{1}{2}(|\beta|^2+|\alpha|^2)}. \quad (3.2.55)$$

Which can be written as

$$\langle \beta | \alpha \rangle = e^{\alpha\beta^* - \frac{1}{2}(|\beta|^2 + |\alpha|^2)}. \quad (3.2.56)$$

Also

$$|\langle \beta | \alpha \rangle|^2 = e^{-(|\alpha|^2 + |\beta|^2) + \alpha\beta^* + \alpha^*\beta} = e^{-|\alpha - \beta|^2}. \quad (3.2.57)$$

The above equation shows that the coherent states are not orthogonal but if $|\beta - \alpha|^2$ is large then they are nearly orthogonal.

The completeness relation

The completeness relation for the coherent state $|\alpha\rangle$ can be written in the form of an integral on to the complex α plane i.e

$$\frac{1}{\pi} \int |\alpha\rangle \langle \alpha| d^2\alpha = 1, \quad (3.2.58)$$

where $d^2\alpha = d\text{Re}(\alpha)d\text{Im}(\alpha)$. The Proof of the above relation is as follows

$$\int |\alpha\rangle \langle \alpha| d^2\alpha = \int e^{-|\alpha|^2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\alpha^n \alpha^{*m}}{\sqrt{n!}\sqrt{m!}} |n\rangle \langle m| d^2\alpha. \quad (3.2.59)$$

We now transform above relation in polar coordinates by taking the explicit form for $\alpha = re^{i\theta}$ such that $d^2\alpha = r dr d\theta$ and get

$$\int |\alpha\rangle \langle \alpha| d^2\alpha = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{|n\rangle \langle m|}{\sqrt{n!}\sqrt{m!}} \int_0^{\infty} dr e^{-r^2} r^{n+m+1} \int_0^{2\pi} d\theta e^{i(n-m)\theta}. \quad (3.2.60)$$

But we know that $\int_0^{2\pi} d\theta e^{i(n-m)\theta} = 2\pi\delta_{nm}$ and by changing the variables as $r^2 = y, 2r dr = dy$ and for the condition that $m = n$ we have

$$\int |\alpha\rangle \langle \alpha| d^2\alpha = \pi \sum_{n=0}^{\infty} \frac{|n\rangle \langle n|}{n!} \int_0^{\infty} dy e^{-y} y^n. \quad (3.2.61)$$

We also know that $\int_0^{\infty} dy e^{-y} y^n = n!$, hence

$$\int |\alpha\rangle \langle \alpha| d^2\alpha = \pi \sum_{n=0}^{\infty} |n\rangle \langle n|. \quad (3.2.62)$$

Which satisfies eq. (3.2.58), by making use of the condition for number state i.e $\sum_{n=0}^{\infty} |n\rangle\langle n| = 1$. By the use of this completeness relation for the coherent state of harmonic oscillator, any arbitrary state vector say $|\varphi\rangle$ in the Hilbert space of harmonic oscillator can be written in terms of the coherent states of harmonic oscillator as

$$|\varphi\rangle = \int \frac{d^2\alpha}{\pi} |\alpha\rangle\langle\alpha|\varphi\rangle. \quad (3.2.63)$$

Over Completeness

A coherent state can be expressed in terms of another coherent state by using the nonorthogonality condition, i.e by making use of eq. (3.2.63)

$$|\beta\rangle = \frac{1}{\pi} \int d^2\alpha |\alpha\rangle\langle\alpha|\beta\rangle, \quad (3.2.64)$$

where $\langle\alpha|\beta\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha^*\beta}$ using eq. (3.2.56).

$$|\beta\rangle = \frac{1}{\pi} \int d^2\alpha e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha^*\beta} |\alpha\rangle. \quad (3.2.65)$$

This relation is referred as over completeness.

Temporal Stability

A coherent state remains coherent under the time evolution. Let us have a coherent state defined at time $t = 0$ as $|\alpha, 0\rangle$. Now the question is, can we get a time evolved coherent state by making use of the coherent state at $t = 0$? The answer is "yes" we can, by making use of the unitary time evolution operator $\hat{U}(t)$ [9]. Such that $\hat{U}(t)|\alpha, 0\rangle = |\alpha, t\rangle$. Where $|\alpha, t\rangle$ is the time evolved coherent state. This operator is defined as

$$\hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}, \quad (3.2.66)$$

where \hat{H} is the usual hamiltonian $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$ for the harmonic oscillator and hence

$$|\alpha, t\rangle = e^{-i\omega t(\hat{a}^\dagger\hat{a} + \frac{1}{2})} |\alpha, 0\rangle. \quad (3.2.67)$$

In previous section we have shown the form of the coherent state $|\alpha\rangle$ in eq. (3.2.25) and eq. (3.2.34). These equations represent the coherent state for harmonic oscillator at time $t = 0$ we may write $|\alpha, 0\rangle$ as

$$|\alpha, 0\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (3.2.68)$$

Now the time evolved state can be written as

$$|\alpha, t\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega t(\hat{a}^\dagger \hat{a} + \frac{1}{2})} |n\rangle. \quad (3.2.69)$$

Also we know that the entity $\hat{a}^\dagger \hat{a}$ is the number operator \hat{N} and $\hat{N}|n\rangle = n|n\rangle$, therefore using these results in above equation we get

$$|\alpha, t\rangle = e^{-\frac{1}{2}|\alpha|^2} e^{-\frac{i\omega t}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega t n} |n\rangle, \quad (3.2.70)$$

Now by defining $\acute{\alpha} = \alpha e^{-i\omega t}$ such that $|\acute{\alpha}| = |\alpha|$, we can write the above equation as

$$|\alpha, t\rangle = e^{-\frac{i\omega t}{2}} \left(e^{-\frac{1}{2}|\acute{\alpha}|^2} \sum_{n=0}^{\infty} \frac{\acute{\alpha}^n}{\sqrt{n!}} |n\rangle \right), \quad (3.2.71)$$

which is again a coherent state only with some time dependent phase factor $e^{-\frac{i\omega t}{2}}$. Therefore a coherent state of harmonic oscillator are stable temporally.

3.3 Generalized Coherent States

So far in this chapter we have discussed the coherent states for harmonic oscillator and some of the properties satisfied by these coherent states. We can also construct the coherent states of the system other than the harmonic oscillator, but this sort of construction demands the complete knowledge of the underlying algebra for the system under consideration. From such algebra we mean the corresponding ladder operators, their commutation relations and much more. We do not always develop such kind of algebra for any arbitrary system, but this does not mean that we can not construct the coherent

states for such cases. We can achieve our target by using the generalized techniques developed for the construction of coherent states for the systems other than the harmonic oscillator.

The early algebra based generalization was introduced by Barut and Girardello in 1971 [10]. Perelomov in 1972 [15] introduced another generalized coherent states called generalized perelomov coherent states, which are applicable to any Lie group. Later in 1996 John R Klauder introduced coherent states for hydrogen atom with out the use of underlying algebra [11]. He purposed a generalized form of states that can be referred as coherent states which are normalized, have the continuity of parameters, resolve unity and possesses temporal stability. Three years after that in 1999 Gazeau and Klauder working together presented a more general criteria for the construction of coherent states for the quantum systems which exhibits discrete and continuous spectra [12]. This technique is the core of our work and we will discuss it in detail in this section. Another generalization was introduced by Fox and Choi in the year 2001 [13]. In their work they have discussed the generalized Gaussian Klauder coherent states of any arbitrary hamiltonian satisfying all of the requirements of the coherent states as set by Gazeau and Klauder [12].

3.3.1 Barut-Girdello Coherent States

Barut-Girardello coherent states were introduced in 1971 in order to generalize the concept of Lie algebra of non compact groups [10]. A connection was developed relating Lie algebra. The generalized coherent states was constructed by considering them as the eigenstates of annihilation operator say L^- . The generalized form of this state is

$$|\xi\rangle = \sqrt{\Gamma(-2l)} \sum_{m=0}^{\infty} \frac{(\sqrt{2}\xi)^m}{(m!(\Gamma(-2l+m)))^{\frac{1}{2}}} |l, m\rangle, \quad (3.3.1)$$

where $|l, m\rangle$ are the basis vector of the Hilbert space and ξ is any complex number.

3.3.2 Perelomove Coherent States

Perelomove in 1972 [15] and presented a more generalized form of the coherent states based on algebraic structure which works for all kinds of Lie algebra. He defined these coherent states as

The system of coherent states which have the form $(D|\psi_0\rangle)$ is called a set of states $|\psi_n\rangle$ i.e $|\psi_n\rangle = D(n)|\psi_0\rangle$ where n runs over all the group G . Let H be the stationary subgroup of the state $|\psi_0\rangle$. then the coherent state $|\psi_n\rangle$ can be determined by the point $x = x(n)$ of the factor space G/H corresponding to the element n i.e $|\psi_n\rangle = e^{i\alpha}|x\rangle$ and $|\psi_0\rangle = |0\rangle$,

where D is the representation of the group G acting in the some space H and $|\psi_0\rangle$ is a fixed vector of this space.

3.3.3 Gazeau-Klauder (G.K) Coherent States

The Algebra independent generalized coherent states were introduced by Klauder in 1996 [11] and the idea was extended in a joint effort by Gazeau and Klauder in 1999 [12]. They named these states as generalized Gazeau-Klauder (G.K) coherent states, that are defined for the quantum systems which exhibits discrete energy spectrum by making use of two coherent state parameters say $|\zeta, \vartheta\rangle$ where $\zeta \geq 0$ and $-\infty < \vartheta < \infty$. In order to call the state $|\zeta, \vartheta\rangle$ they also have mentioned a set of suitable requirements involving the Hamiltonian operator \hat{H} for the concerned quantum system. These requirements are as follows

1. Continuity of the parameters i.e $(\acute{\zeta}, \acute{\vartheta}) \rightarrow (\zeta, \vartheta)$.
2. Resolution of unity i.e $1 = \int |\zeta, \vartheta\rangle\langle\zeta, \vartheta|dx(\zeta, \vartheta)$.
3. Temporal stability i.e $exp(-i\hat{H}t)|\zeta, \vartheta\rangle = |\zeta, \vartheta + \omega t\rangle$ ω is a constant.
4. Action Identity i.e $\langle\zeta, \vartheta|\hat{H}|\zeta, \vartheta\rangle = \omega\zeta$.

For any Hamiltonian say \hat{H} having a discrete spectrum with the condition that $\hat{H} \geq 0$ and $\hat{H}|n\rangle = E_n|n\rangle$ where $n \geq 0$ and $|n\rangle$ are orthonormal eigenstates of \hat{H} the generalized G.K coherent states can be defined as

$$|\zeta, \vartheta\rangle = \frac{1}{\sqrt{N(\zeta)}} \sum_{n=0}^{\infty} \frac{\zeta^{\frac{n}{2}} e^{-ie_n\vartheta}}{\sqrt{\rho_n}} |n\rangle, \quad (3.3.2)$$

where e_n is the dimensionless form of the energy spectrum E_n and ρ_n is defined as the product of these dimensionless energies e_n i.e

$$\rho_n = \prod_{i=0}^n e_i, \quad (3.3.3)$$

In order for this product to be non zero we set the energy for ground state $e_0 = 1$. $N(\zeta)$ is the normalization constant which can be chosen so that

$$\langle \zeta, \vartheta | \zeta, \vartheta \rangle = \frac{1}{N(\zeta)} \sum_{n=0}^{\infty} \frac{\zeta^n}{\rho_n} \equiv 1, \quad (3.3.4)$$

Therefore

$$N(\zeta) = \sum_{n=0}^{\infty} \frac{\zeta^n}{\rho_n}. \quad (3.3.5)$$

These generalized states can readily be reduced to the coherent states for the harmonic oscillator. For the harmonic oscillator the energy spectrum can be given as $E_n = \hbar\omega(n + \frac{1}{2})$. We can write its dimensionless form as $e_n = n$ with out the loss of generality. Now making use of eq. (3.3.3) we can write $\rho_n = n!$. Also we may assume that $\alpha = \sqrt{\zeta} e^{-i\vartheta}$ such that $\alpha^n = \zeta^{\frac{n}{2}} e^{-in\vartheta}$ also by eq. (3.3.5) the normalization constant $N(\zeta)^2 = e^\zeta$ which can be written in the form of α as $N(\zeta) = e^{\frac{1}{2}|\alpha|^2}$ by substituting these values in eq. (3.3.2) we get

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (3.3.6)$$

which is exactly in accordance with the eq. (3.2.25) and eq. (3.2.34). We may also say that these generalized G.K coherent states are actually the generalized form of the harmonic oscillator coherent states.

Applications of G.K Coherent States

Generalization of coherent states makes them very useful in different fields of Physics. Coherent states are of fundamental importance in the field of quantum optics. For example generalized G.K coherent states were developed for pseudo-harmonic oscillator [18], the Morse potential [23,24], Pöschl-Teller potential [19], the power law potentials [20,21], the triangular well potential [22]. These coherent states can be used to discuss anharmonic crystals [42], non equilibrium statistical mechanics [43], elementary particle physics [44,45], quantum oscillators [48] and many more applications of coherent states can be found in [46,47].

3.3.4 Gaussian Klauder Coherent States

The generalized Gaussian coherent states [14] were introduced by R. Fox in the year 1999. These states were introduced in order to criticise the notion that a Gaussian function can not be used to approximate a coherent state. Fox presented that a Gaussian function is quite suitable choice for the construction of generalized Gaussian coherent states and he clearly mentioned that these states resolve unity and shows a little variation for the selected operators. He constructed these states for harmonic oscillator and Rydberg atom. He named these states as Gaussian-Klauder coherent states and constructed them for a particle in 2D square box [13]. The Generalized form for such states can be written as

$$|\zeta, \vartheta\rangle = \sum_{n=0}^{\infty} \frac{e^{-\frac{(n-\zeta)^2}{4\sigma^2}}}{(N(\zeta))^{\frac{1}{2}}} e^{ie_n\vartheta} |n\rangle, \quad (3.3.7)$$

Where $N(\zeta)$ is the normalization constant and is given as

$$N(\zeta) = \sum_{n=0}^{\infty} e^{-\frac{(n-\zeta)^2}{2\sigma^2}}. \quad (3.3.8)$$

Also ζ and ϑ are the coherent state parameters such that $\zeta \geq 0$ and $-\infty < \vartheta < \infty$ and σ is related to the width of the Gaussian.

Chapter 4

The Coherent States for the Morse Oscillator

4.1 Introduction

After discussing the Morse oscillator in chapter 2 and developing the concepts about the coherent states for general systems in chapter 3, we are now in a position to develop the coherent states for the Morse oscillator. The formalism introduced by Gazeau and Klauder (*hereafter referred to as G-K*) for the construction of coherent states [12] for the general hamiltonian is quite suitable for the Morse oscillator. Earlier some attempts have been made [23, 31, 32] by various authors to construct the coherent states for the Morse oscillator. In present work we construct the coherent states for the Morse oscillator using G-K formalism and discuss their dynamical behaviour by means of auto correlation function, position and momentum space wavefunctions and the Wigner distribution function.

The chapter is organized as follows: In section 4.2 the G-K coherent states for the Morse oscillator are constructed. The statistical measures which are necessary for the study of the coherent states are discussed in section 4.3. Section 4.4 is dedicated to the study of the dynamical behaviour of these states. We calculate the auto correlation function and study the phenomenon of quantum revivals. We construct the coherent state wave packets

in position space and momentum space, and discuss their time dependence. Then the position and momentum space probability densities are calculated as a function of time that leads to the formation of the quantum carpets. Moreover, we calculate the expectation values of position and momentum and discuss the phase space spanned by these expectation values. Lastly we discuss Wigner quasi probability distribution function. The Wigner function accounts for the nonclassical characteristics of the Morse oscillator.

4.2 Gazeau-Klauder Coherent States for Morse Oscillator

Following the G-K formalism, presented in chapter 3, the coherent states for the Morse oscillator can be given as

$$|\zeta, \vartheta\rangle = \frac{1}{\sqrt{N(\zeta)}} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{n}{2}} e^{-ie_n \vartheta}}{\sqrt{\rho_n}} |n\rangle, \quad (4.2.1)$$

where e_n is the dimensionless form of energy spectrum which we can calculate using the expression for energy spectrum E_n eq. (2.3.19) as

$$e_n \equiv \kappa(E_n - E_0) = -n(n+1-\nu), \quad (4.2.2)$$

where $\kappa = -\frac{2\mu}{\hbar^2 \xi^2}$, E_n is the energy of the n^{th} state and E_0 is the energy of the ground state. Also ρ_n is defined by eq. (3.3.3) as the product of the above dimensionless energy spectrum e_n , where $\rho_0 = 1$. We can get an explicit form of ρ_n by making use of eq. (4.2.2) in eq. (3.3.3)

$$\rho_n \equiv \prod_{i=1}^{n_{max}} e_i = n! \frac{\Gamma(\nu-1)}{\Gamma(\nu-n-1)}, \quad (4.2.3)$$

while deriving the above expression we make use of the following property of the gamma function i.e,

$$\Gamma(z) = \frac{\pi}{\text{Sin}(\pi z)} \frac{1}{\Gamma(1-z)}. \quad (4.2.4)$$

From eq. (4.2.2) we can see that due to the presence of the factor ν energy spectrum can not take infinite values. Therefore the summation on n in eq. (4.2.1) does not run from 0 to ∞ , but up to some finite number which can be determined using eq. (2.4.6) as $n_{max} = \frac{\nu-1}{2}$. Where $N(\zeta)$ is the normalization constant given by eq. (3.3.5) and explicitly given for the Morse oscillator as

$$N(\zeta) = \sum_{n=0}^{n_{max}-1} \frac{\zeta^n \Gamma(\nu - n - 1)}{n! \Gamma(\nu - 1)}. \quad (4.2.5)$$

Also ζ and ϑ are real parameters. The domain of ϑ is $-\infty < \vartheta < \infty$ while ζ lies between $0 < \zeta < R$ and R is the radius of convergence and depend upon the nature of ρ_n at large value of n and is given as $R = \lim_{n \rightarrow \infty} \sqrt[n]{\rho_n}$.

It can be proved that the coherent state given by the eq. (4.2.1) satisfies all of the requirements set by Gazeau and Klauder i.e continuity of parameters, temporal stability and action identity, while the resolution of unity is still an open problem for the case of Morse potential. We can take resolution of unity for granted and study the dynamical properties of the coherent state for the Morse oscillator.

4.3 Statistical Measures of the Coherent State

Before presenting the dynamics of the states constructed for the Morse oscillator, here we want to mention some of the statistical measures of the coherent state. The statistical measures involves the calculation of 1st and 2nd order expectation values of the number operator \hat{N} .

$$\langle n \rangle = \langle \zeta, \vartheta | \hat{N} | \zeta, \vartheta \rangle = \sum_{n=0}^{n_{max}-1} \frac{1}{N(\zeta)} \frac{n \zeta^n}{\rho_n}, \quad (4.3.1)$$

$$\langle n^2 \rangle = \langle \zeta, \vartheta | \hat{N}^2 | \zeta, \vartheta \rangle = \sum_{n=0}^{n_{max}-1} \frac{1}{N(\zeta)} \frac{n^2 \zeta^n}{\rho_n}. \quad (4.3.2)$$

Using the above expectation values we can define the spread of number operator Δn as

$$\Delta n = \sqrt{\langle n^2 \rangle - \langle n \rangle^2}. \quad (4.3.3)$$

The calculation of mean and Δn is essential, as the weighting distribution of the coherent states depends upon these entities. For example in the case of coherent states for the harmonic oscillator the mean and spread Δn are equal which characterizes a poisson distribution. For the case of coherent states for the triangular well [22] the spread is always greater than mean hence the weighting distribution is super-Poissonian. The weighting distribution for the above coherent states can be defined as

$$|w_n|^2 \equiv |\langle n|\zeta, \vartheta\rangle|^2 = \frac{1}{N(\zeta)} \frac{\zeta^n}{\rho_n}, \quad (4.3.4)$$

where w_n accounts for the initial localization of the coherent state around $\langle n \rangle$. The weighting distribution is dependent on the coherent state parameter ζ , in such a way that $\langle n \rangle$ changes with ζ . This dependence is illustrated by the following figure 4.1

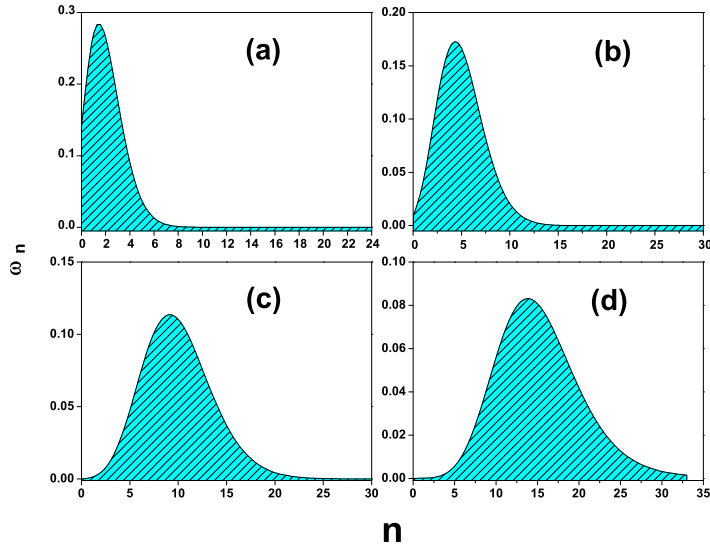


Figure 4.1: Dependence of $\langle n \rangle$ on the Model Parameter ζ in (a) $\zeta = 106$, $\langle n \rangle \approx 2$, (b) $\zeta = 251$, $\langle n \rangle \approx 5$, in (c) $\zeta = 451$, $\langle n \rangle \approx 10$ and in (d) $\zeta = 602$, $\langle n \rangle \approx 15$, also for numerics we have taken $\xi = 0.5$, $\vartheta \approx 0$, $\nu = 57.44$ and $n_{max} = 27$.

4.4 Dynamical Behaviour of the Coherent State

In previous section we have seen the construction of the coherent states for the Morse oscillator along with the various parameters involved. This section is dedicated to the study of the dynamical behaviour of these states.

4.4.1 Time Evolution of the Coherent State

The time evolved coherent state can be obtained by the action of the time evolution operator $\hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}$ on eq. 4.2.1 as $\hat{U}(t)|\zeta, \vartheta\rangle = |\zeta, \vartheta, t\rangle$ and time dependent form can be written as

$$|\zeta, \vartheta, t\rangle = \frac{1}{\sqrt{N(\zeta)}} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{n}{2}} e^{-ie_n(\vartheta + \frac{\omega t}{2})}}{\sqrt{\rho_n}} |n\rangle, \quad (4.4.1)$$

where ω is the phase frequency and \hat{H} is the Hamiltonian for the Morse oscillator. We are intrusted in the temporal characteristics of these states. In other words, we are intrusted to find out how closely the time evolved states resembles to the initial states. Which can be explained by the auto correlation function.

Auto Correlation Function $A(t)$

According to Poincarè's theorem, the states of the quantum system which have the discrete energy eigenvalues and are initially localized, when evolved with time eventually regain its initial form. This phenomenon can be observed using the auto correlation function [49] and the time elapsed in this interval is known as revival time [49–51]. The time development of the coherent state given by eq. (4.4.1) involves the study of the overlap $\langle \zeta, \vartheta, t | \zeta, \vartheta, 0 \rangle$. This overlap is termed as auto correlation function $A(t)$ and can be written as

$$A(t) \equiv \langle \zeta, \vartheta, t | \zeta, \vartheta, 0 \rangle = \langle \zeta, \vartheta | e^{-\frac{i\hat{H}t}{\hbar}} | \zeta, \vartheta \rangle, \quad (4.4.2)$$

where, \hat{H} is hamiltonian of the system under consideration. This overlap is also used to calculate the time which the system took to reach an orthogonal

quantum state, called the time of revival. Using eq. (4.2.1) and the relation $\hat{H}|n\rangle = E_n|n\rangle$ we can write eq. (4.4.2) as

$$A(t) \equiv \langle \zeta, \vartheta, t | \zeta, \vartheta, 0 \rangle = \sum_{n=0}^{n_{max}-1} |w_n|^2 e^{\frac{-iE_n t}{\hbar}}, \quad (4.4.3)$$

where w_n is the weighting distribution given by eq. (4.3.4).

If our coherent state is initially localized around $\langle n \rangle$ having the dispersion $\Delta n \ll \langle n \rangle$, we can take the Taylor expansion of the energy E_n around $\langle n \rangle$ such that

$$E_n = E_{\langle n \rangle} + \frac{1}{1!} \left(\frac{\partial E_n}{\partial n} \right)_{n=\langle n \rangle} (n - \langle n \rangle) + \frac{1}{2!} \left(\frac{\partial^2 E_n}{\partial n^2} \right)_{n=\langle n \rangle} (n - \langle n \rangle)^2 + \dots \quad (4.4.4)$$

The first term in the expansion is independent of n , also such phase factor is common to all the terms in the expansion. Therefore it is unimportant here. The proceeding terms are of great importance as each of them is related to a time scale as

$$T_1 = \frac{2\pi}{\left| \frac{\partial E_n}{\partial n} \right|_{n=\langle n \rangle}}, \quad T_2 = \frac{\pi}{\left| \frac{\partial^2 E_n}{\partial n^2} \right|_{n=\langle n \rangle}}, \dots \quad (4.4.5)$$

Therefore we can define a general formula [20] for time scale as

$$T_\alpha = \frac{2\pi}{\left(\frac{1}{\alpha!} \left| \frac{\partial^\alpha E_n}{\partial n^\alpha} \right|_{n=\langle n \rangle} \right)}, \quad (4.4.6)$$

where

- $\alpha = 1$ corresponds to time of classical period of oscillation T_{cl} .
- $\alpha = 2$ corresponds to quantum revival time T_{qr} .
- $\alpha = 3$ corresponds to super revival time T_{sr} .
- and so on depending upon the n^{th} dependence of e_n .

Particularly for the Morse oscillator this time scale is only restricted to the quantum revival time as the energy spectrum E_n eq. (2.3.19) is of the order n^2 and the higher order derivatives of E_n vanish. The time for classical period T_{cl} and quantum revival T_{qr} for the case of Morse oscillator can be found by taking 1st and 2nd derivative of eq. (4.2.2) with respect to n i.e,

$$\frac{\partial E_n}{\partial n} = \frac{\xi^2}{2}(-2n - \nu + 1), \quad \frac{\partial^2 E_n}{\partial n^2} = \frac{\xi^2}{2}(-2). \quad (4.4.7)$$

By making use of eq. (4.4.6) and $\alpha = 1$ we get the expression for T_{cl} as,

$$T_{cl} = \frac{4\pi}{\xi^2|-2\langle n \rangle - \nu + 1|}, \quad (4.4.8)$$

also the expression for T_{qr} using $\alpha = 2$ is,

$$T_{qr} \equiv \frac{4\pi}{\xi^2} = |-2\langle n \rangle - \nu + 1|T_{cl}. \quad (4.4.9)$$

While analysing the statistical measures we have specified that the mean value $\langle n \rangle$, of the weighting distribution has a direct dependance of the coherent state parameter ζ . This implies that the time for classical period and quantum revival also have an inverse dependence upon the coherent state parameter ζ by virtue of eq. (4.4.6). However for the case of the Morse oscillator having an energy spectrum which have a quadratic dependence upon n , this makes T_{qr} independent of $\langle n \rangle$ and therefore have no dependence on ζ . Due to the inverse dependence of T_{cl} on ζ , we conclude that if we increase the value of ζ the number for classical periods increases in quantum revival of the coherent state. This feature can also be observed in the following figure 4.2 for the modulus square of auto correlation function.

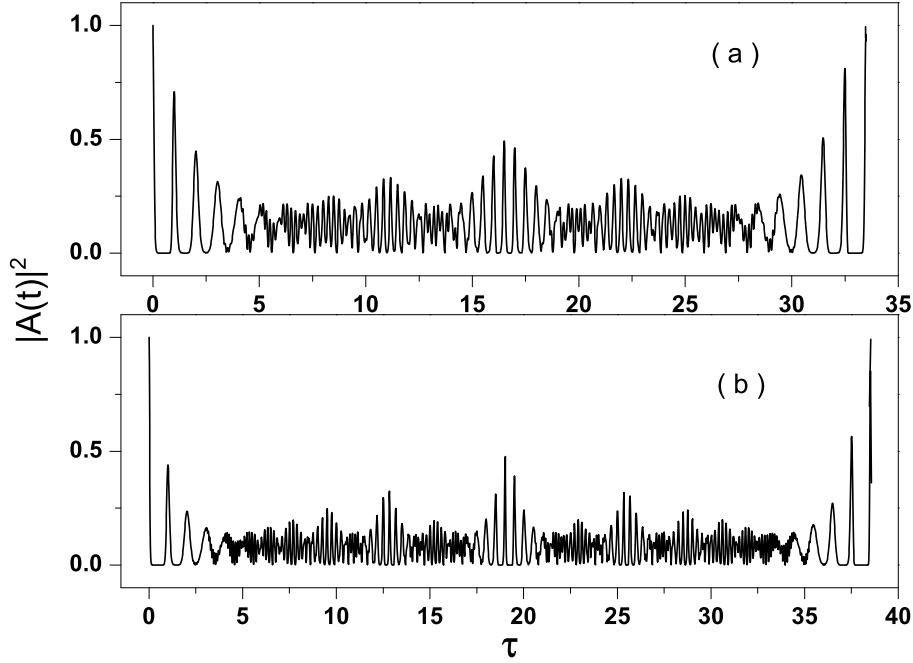


Figure 4.2: Modulus square of auto correlation function (a) for $\langle n \rangle = 5$ and (b) for $\langle n \rangle = 10$.

Here, from these graphs we can clearly see the exact meaning of the quantum revival. It can be noticed that at $t = 0$ the overlap $\langle \zeta, \vartheta, t | \zeta, \vartheta, 0 \rangle$ give maximum result, but after few classical periods this overlap undergoes a collapse. In the middle region, we see some sort of fractional revivals, but with the passage of some more time this overlap again give maximum value, this time is named as quantum revival time. Also similar kind of plots can be found in [20] for harmonic oscillator restricted only to classical period, Infinite square well restricted to quantum revival time and the triangular well potential with no bounds on the time scale depending on the n^{th} dependence of the corresponding energy spectrum E_n .

4.4.2 Dynamics In Position Space

Position Space Wave Function

The position space time dependent wave function $\Psi(x, \zeta, \vartheta, t)$ for G.K coherent state for the Morse potential can be written by projecting a position bra i.e $\langle x|$ on to the coherent state given by eq. (4.4.1)

$$\Psi(x, \zeta, \vartheta, t) \equiv \langle x|\zeta, \vartheta, t\rangle = \frac{1}{\sqrt{N(\zeta)}} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{n}{2}} e^{-ie_n(\vartheta + \frac{\omega t}{2})}}{\sqrt{\rho_n}} \langle x|n\rangle, \quad (4.4.10)$$

where, $\langle x|n\rangle$ is the eigenfunction $\psi_n(x)$ for morse potential as given by eq. (2.3.17). Hence our coherent state in position representation can be written as

$$\Psi(x, \zeta, \vartheta, t) = \frac{1}{\sqrt{N(\zeta)}} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{n}{2}} e^{-ie_n(\vartheta + \frac{\omega t}{2})}}{\sqrt{\rho_n}} \psi_n(x). \quad (4.4.11)$$

The dependence of probability distribution $|\Psi(x, \zeta, \vartheta, t)|^2$ on the coherent state parameter ζ taking $\vartheta = 0$ and $t = 0$ can be shown in the Figure 4.3. From the figure we conclude that with increasing the value of the parameter ζ the center of the initial state shift towards left and results in the delocalization of the probability distribution in space, as the height of the decreases and width increases.

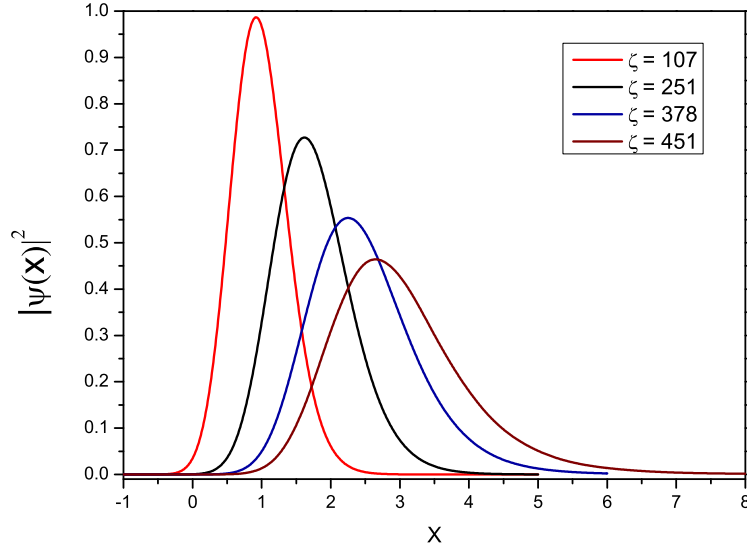


Figure 4.3: Probability distribution dependence on the coherent state parameter ζ at $t = 0$.

Time Evolution of Probabilities Densities

The snap shots for probability density at different intervals of time can be represented by following figure. In this figure we see that for a fixed value of ζ which we have taken as 251 for present case. At $t = 0$ we get a single well localized peak, as time passes this peak splits up in to multiple peaks and gets delocalized in space this can be observer at $t = 5T_{cl}$ and at $t = 15T_{cl}$, but at the revival time we again get a single well localized peak resembling the one we have obtained at $t = 0$.

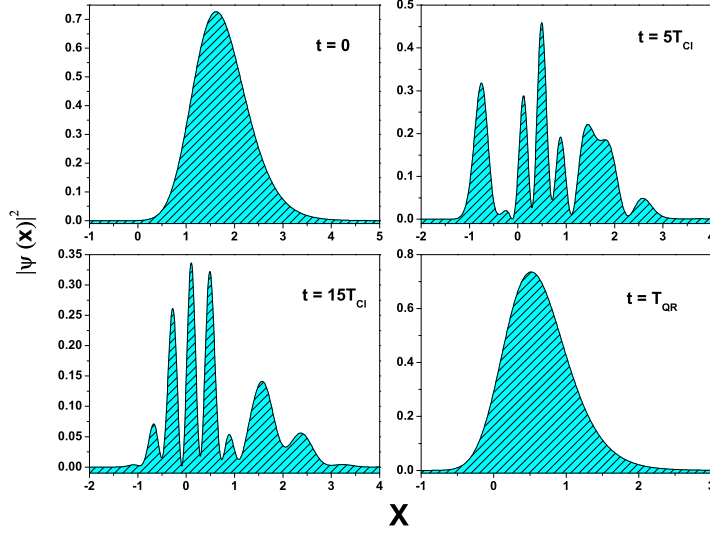


Figure 4.4: Snap shots for probability density at different times.

We can also study the evolution of probability density as a function of time by plotting the quantum carpets for position space wave function, for the coherent states of the Morse potential Figure 4.5. The probability density is defined as

$$|\Psi(x, \zeta, \vartheta, t)|^2 = \Psi^*(x, \zeta, \vartheta, t)\Psi(x, \zeta, \vartheta, t), \quad (4.4.12)$$

which on using eq. (4.4.11) becomes

$$|\Psi(x, \zeta, \vartheta, t)|^2 = \frac{1}{N(\zeta)} \sum_{m=0}^{n_{max}-1} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{m+n}{2}}}{\sqrt{\rho_m}\sqrt{\rho_n}} e^{-i(e_n-e_m)(\vartheta+\frac{\omega t}{2})} \psi_m^*(x)\psi_n(x). \quad (4.4.13)$$

The above expression can be split in to two expression which are,

$$x_1 = \frac{1}{N(\zeta)} \sum_{m=n} \frac{J^n}{\rho_n} |\psi_n(x)|^2, \quad (4.4.14)$$

$$x_2 = \frac{1}{N(\zeta)} \sum_{m \neq n} \frac{J^{\frac{n+m}{2}}}{\sqrt{\rho_n}\sqrt{\rho_m}} e^{-i(e_n-e_m)(\vartheta+\frac{\omega t}{2})} \psi_m^*(x)\psi_n(x). \quad (4.4.15)$$

Hence eq. (4.4.13) becomes,

$$|\Psi(x, \zeta, \vartheta, t)|^2 = x_1 + x_2. \quad (4.4.16)$$

It can be concluded that the expression for x_1 is independent of time and therefore provides us with a constant back ground in the formation of quantum carpets. While on the other hand x_2 is dependent upon time and results in the quantum interfering terms which result in the formation of the pattern we observe in figure 4.5. The colored region in Figure 4.5 represents the max-

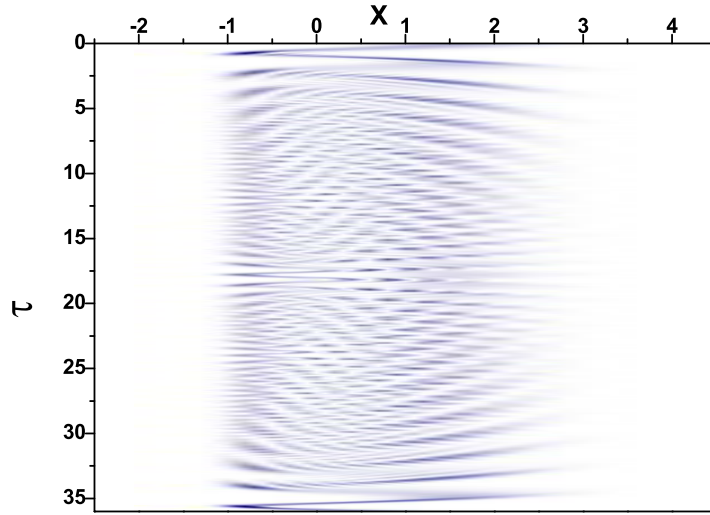


Figure 4.5: Quantum carpet for one T_{gr} with $\zeta = 251$.

imum probabilities while the white space represents minimum probabilities. For the comparison we also plotted the quantum carpet for $\frac{1}{4}T_{gr}$ along with the quantum carpet for harmonic oscillator in position space. We can see that for few classical periods these carpets shows similar trend, but as time increases the quantum carpet for Morse oscillator become distorted due to the quantum interferences representing anharmonic behaviour. On the other hand the quantum carpet for harmonic oscillator runs smoothly showing the harmonic behaviour.

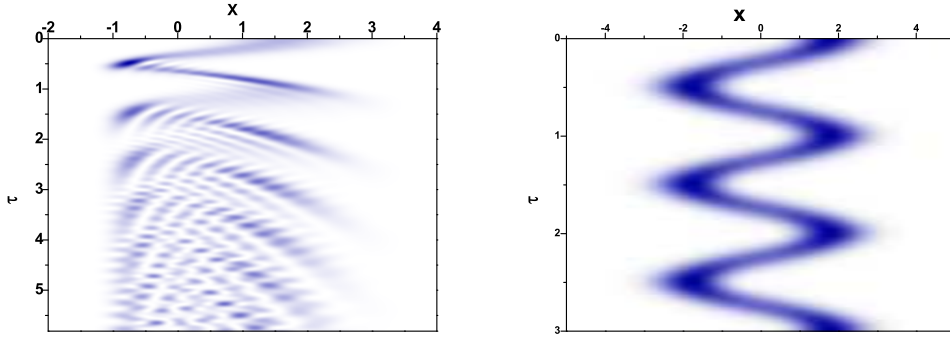


Figure 4.6: Graphical comparison between the quantum carpet for coherent state of Morse oscillator and harmonic oscillator.

4.4.3 Dynamics in Momentum Space

The Momentum Space Wave Function

The Fourier Transform connects the position space wave function to the momentum space wave function by the following relation

$$\phi_n(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ip \cdot x}{\hbar}} \psi_n(x) dx. \quad (4.4.17)$$

So our coherent state wave function for the Morse oscillator in momentum space can be written as

$$\Phi(p, \zeta, \vartheta, t) = \frac{1}{\sqrt{N(\zeta)}} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{n}{2}}}{\sqrt{\rho_n}} e^{-ie_n(\vartheta + \frac{\omega t}{2})} \phi_n(p). \quad (4.4.18)$$

The dependence of probability density $|\Phi(p, \zeta, \vartheta, t)|^2$ on the model parameter ζ in momentum space is shown in Figure 4.7. Here we also take $\vartheta = 0$ and $t = 0$. From the figure 4.7, an opposite trend compared to position space has been noted for momentum space. In this case, we have established that as ζ increases the probability distribution of the momentum space wavefunction gets more localized. This comparison is in agreement with the Heisenberg uncertainty relationship.

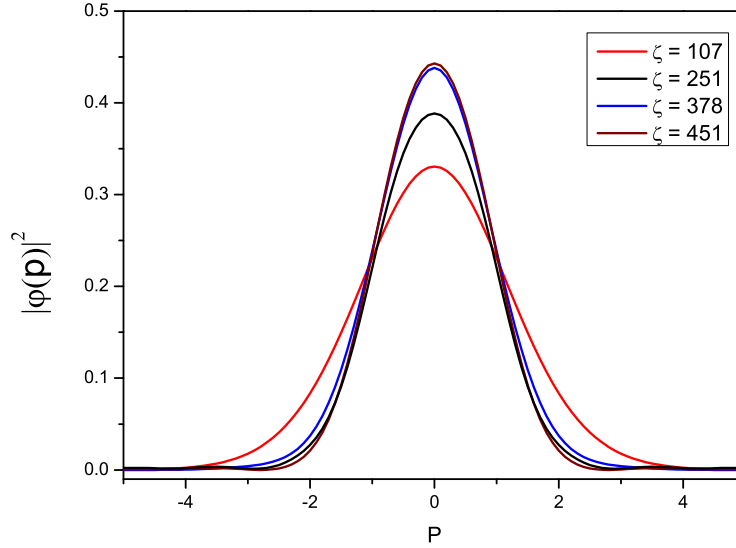


Figure 4.7: Probability density dependence on the coherent state parameter ζ at $t = 0$.

Time Evolution of Probabilities Densities

The snap shots for probability density at different intervals of time can be represented by the following Figure 4.4.3. Here, a similar behavior as has been observed as for position space wave packet. For $\zeta = 251$ and at $t = 0$ we got a well localized probability density; as time passes the single peak splits up into multiple peaks and get delocalized in space. This can also be observed at $t = 5T_{cl}$ and at $t = 15T_{cl}$. We witnessed a well localized peak at the revival time $t = T_{qr}$.

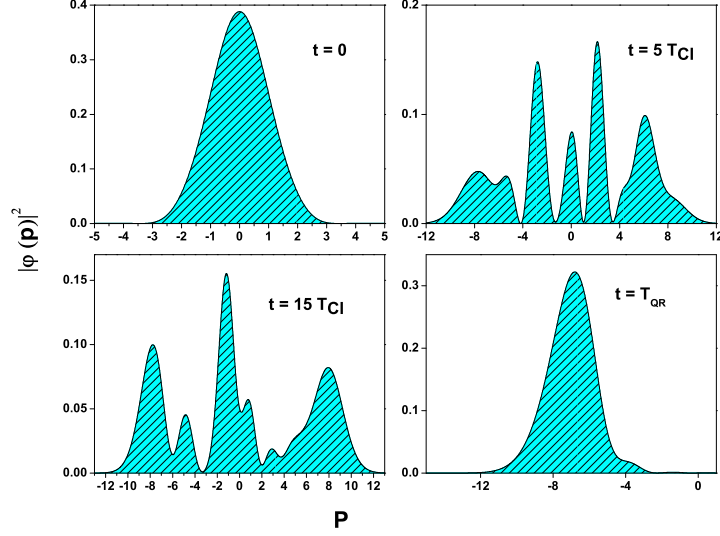


Figure 4.8: Snap Shots of Probability density at Different Times.

The complete picture for the time evolution of the probability density can be shown by using the quantum carpet for momentum space using eq. (4.4.18). The probability density for momentum space is defined as

$$|\Phi(p, \zeta, \vartheta, t)|^2 = \Phi^*(p, \zeta, \vartheta, t)\Phi(p, \zeta, \vartheta, t), \quad (4.4.19)$$

which on using eq. (4.4.18) can be written as

$$|\Phi(p, \zeta, \vartheta, t)|^2 = \frac{1}{N(\zeta)} \sum_{m=0}^{n_{max}-1} \sum_{n=0}^{n_{max}-1} \frac{\zeta^{\frac{m+n}{2}}}{\sqrt{\rho_m}\sqrt{\rho_n}} e^{-i(e_n-e_m)(\vartheta+\frac{\omega t}{2})} \phi_m^*(p)\phi_n(p). \quad (4.4.20)$$

The above expression can also be written in the form of two summations as we have previously for the case of position space wavepacket.

$$p_1 = \frac{1}{N(\zeta)} \sum_{m=n} \frac{J^n}{\rho_n} |\phi_n(p)|^2, \quad (4.4.21)$$

$$p_2 = \frac{1}{N(\zeta)} \sum_{m \neq n} \frac{J^{\frac{n+m}{2}}}{\sqrt{\rho_n}\sqrt{\rho_m}} e^{-i(e_n-e_m)(\vartheta+\frac{\omega t}{2})} \phi_m^*(p)\phi_n(p). \quad (4.4.22)$$

Such that eq. (4.4.20) becomes,

$$|\Phi(p, \zeta, \vartheta, t)|^2 = p_1 + p_2. \quad (4.4.23)$$

Figure 4.9 shows the quantum carpet for one T_{qr} for Momentum space and

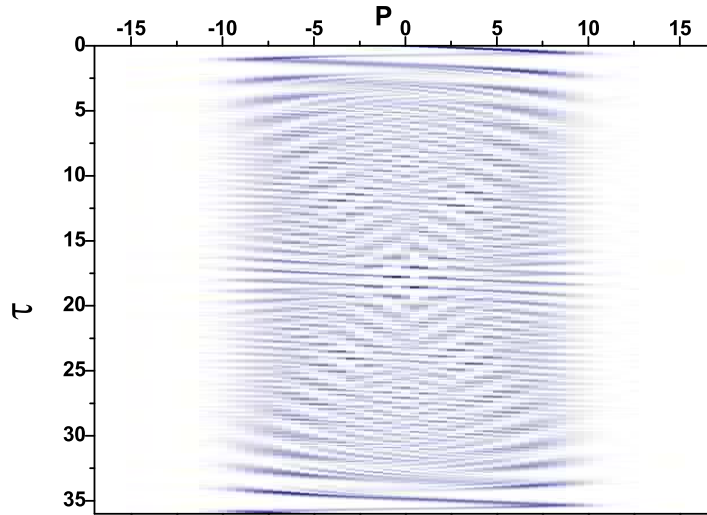


Figure 4.9: Quantum Carpet for one T_{qr} with $\zeta = 251$.

all other parameters are same as we have used for the calculation of position space quantum carpet. The similar result can be concluded from this picture as we got in the case of position space. The time independent term p_1 provides a constant back ground while time dependent term p_2 is responsible for the quantum interferences. Like before here we show a comparison between quantum carpet of Morse oscillator for $\frac{1}{4}T_{qr}$ and quantum carpet of harmonic oscillator as we have shown in the position space representation. Here we also see the similar behaviour as we have discussed before for position space.

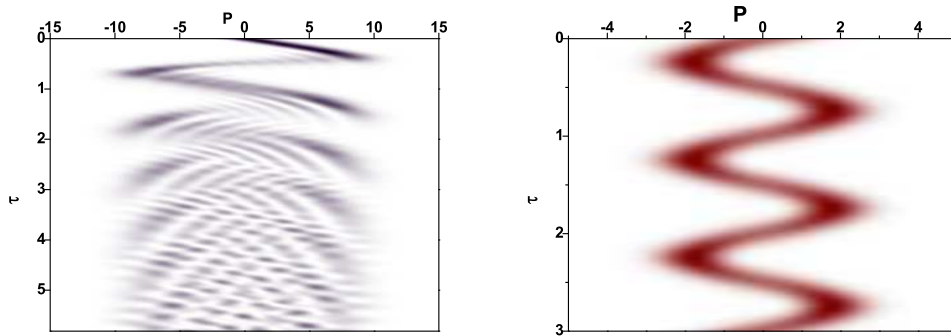


Figure 4.10: Graphical comparison between the quantum carpet for coherent state of Morse oscillator and Harmonic oscillator.

4.4.4 The Phase Space Picture

Time Evolution of Expectation Values $\langle x(t) \rangle$

The time dependent coherent state wave function for the Morse oscillator is given by eq. (4.4.11). We can study the time evolution of the expectation values of position by using formula

$$\langle x(t) \rangle = \int_{-\infty}^{\infty} x |\Psi(x, \zeta, \vartheta, t)|^2 dx \quad (4.4.24)$$

Time evolution of the expectation values in position space for one quantum revival time T_{qr} is shown in Figure 4.11. For the numerics we have used eq. (4.4.11) taking $\zeta = 251$, $\vartheta = 0$, $\xi = 0.5$, $\nu = 57.44$, $n = 0, 1, \dots, 27$, $\langle n \rangle = 5$ and taking integrating limits from $x = 0, 1, \dots, 10$. From Figure 4.11 we see the trend with which the expectation values of position are evolving with time. The average values dies in the middle but reappears at quantum revival time.

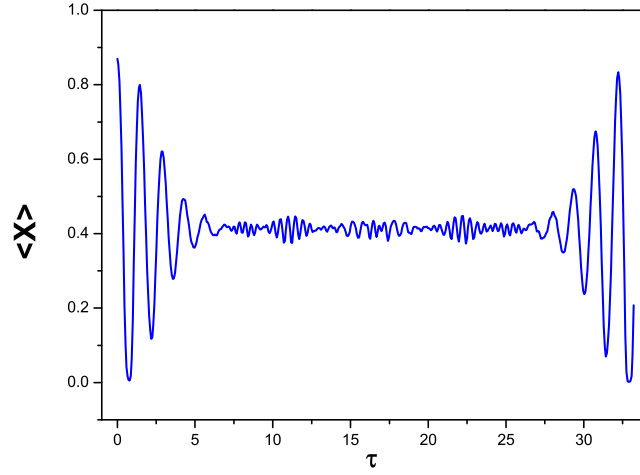


Figure 4.11: Expectation values for T_{qr} , $\tau = \frac{t}{T_{cl}}$.

Time Evolution of Expectation Values $\langle p(t) \rangle$

Using eq. (4.4.18) we are able to find the time evolution of the expectation values of momentum.

$$\langle p(t) \rangle = \int_{-\infty}^{\infty} p |\Phi(p, \zeta, \vartheta, t)|^2 dp. \quad (4.4.25)$$

The plot for eq. (4.4.25) is given in figure 4.12. For numerics we have used same values as we have used for the case of expectation values of position. Here we have taken the integrating limits for momentum $p = 0, 1, \dots, 10$. From Figure 4.12, we see the trend about the time evolution of the expectation values which also dies in the middle and revive again at revival time T_{qr} .

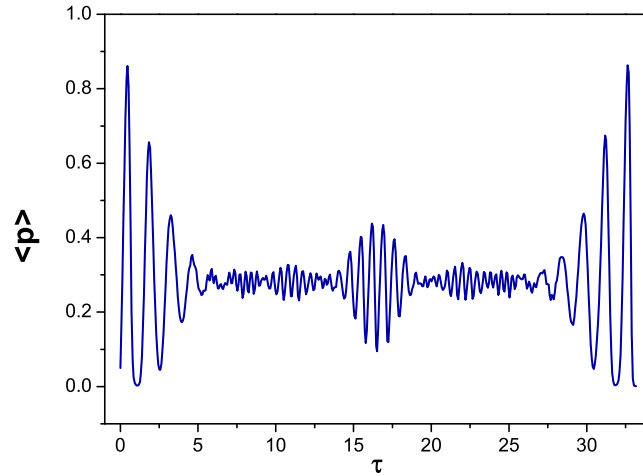


Figure 4.12: Plot for $\langle p \rangle$ for one T_{qr} with $\zeta = 251$, $\tau = \frac{t}{T_{cl}}$.

We have calculated the expectation values in position space $\langle x(t) \rangle$ and as well as in momentum space $\langle p(t) \rangle$. Now by using these expectation values we are going to present a Phase Space picture Figure 4.13 representing the time evolution for one T_{qr} of the Morse oscillator. From this figure it can be noted that initially for few classical periods we get approximately a closed trajectory as one can observe for the case of harmonic oscillator. But as time passes and the quantum interferences arises, we get a spiral phase space trajectory which minimizes with time till we see some fractional revivals in the middle. After these fractional revivals it again minimizes with time. As we approach near quantum revival the trajectory again gets maximize full revival can be observed at revival time T_{qr} .

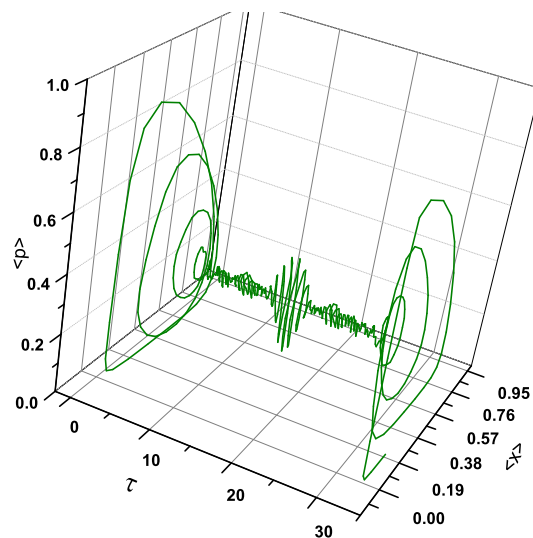


Figure 4.13: phase space for one T_{qr} with $\zeta = 251$.

4.4.5 Quasi Probability Distribution

In past due to the increasing development in the field of quantum mechanics science society felt a need to calculate the quantum mechanical behaviour of the system in a classical way. The first milestone in this regard is the phase space distribution. In order to measure the expectation values of quantum mechanical observable in classical fashion Wigner in the year 1932 introduced the Wigner distribution function by considering the joint distribution of the probabilities in momentum and position space. This distribution function took much fame as it involves the features that are common to both classical mechanics and quantum mechanics. This Wigner distribution takes on the negative values which makes it different form the probability distribution that will always give us positive values. So it is named as quasi probability distribution. The reason for the appearance of these negative values was efficiently discussed in [53] by Hudson In his work he mentioned that Wigner distribution function involves the observable X for position and P for momentum satisfying the Heisenberg commutation relation $[X, P] = i\hbar$. Incompatibility of these observables is the reason for the appearance of these negative prob-

abilities. Due to the incompatibility joint probability distribution can not be measured by any experimental technique which is a postulate of quantum theory. We can therefore also refer the appearance of the negative values as the appearance of non classicality of the quantum system under study. In [54] Tatarski discussed the specific rules and properties which makes this quasi probability distribution different form the true probability.

For our coherent state wave function given in eq. (4.4.10) the Wigner function can be defined as

$$W(x, p) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \Psi^*(\zeta, x - \frac{1}{2}z, 0) \Psi(\zeta, x + \frac{1}{2}z, 0) e^{\frac{ipz}{\hbar}} dz. \quad (4.4.26)$$

Here, we have plotted Wigner function for different values of ζ . Form these plots it is evident that for smaller value of ζ non classicality is minimum but as we increase the value of ζ the non classicality becomes more and more prominent.

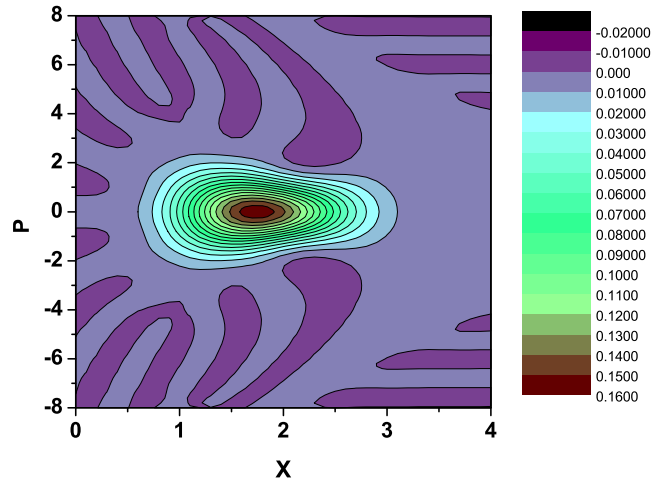
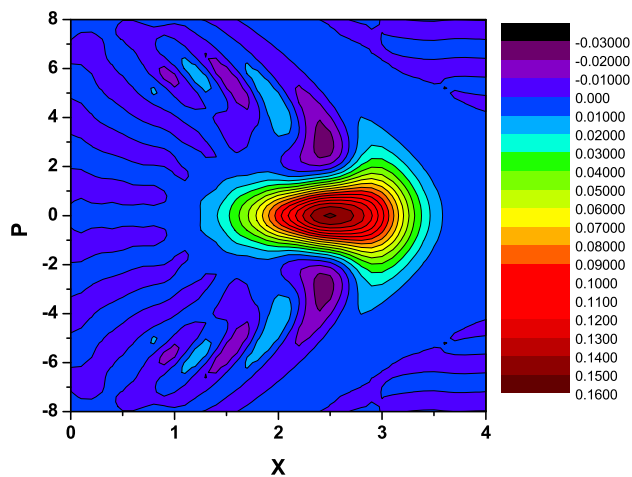
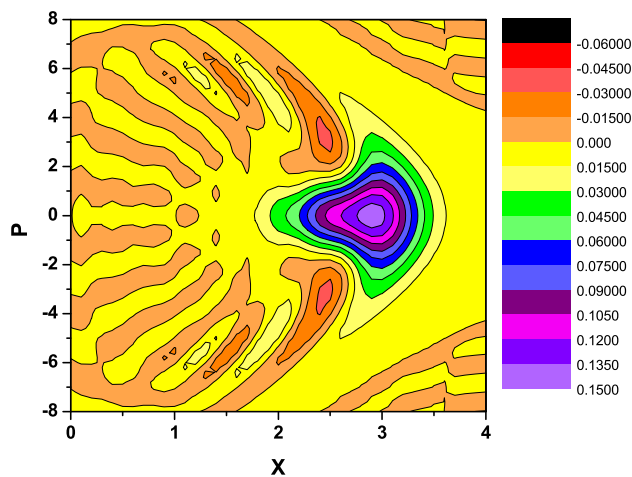


Figure 4.14: Contour plot of wigner function for $\zeta = 251$.

Figure 4.15: Contour plot of wigner function for $\zeta = 452$.Figure 4.16: Contour plot of wigner function for $\zeta = 602$.

Chapter 5

Summary and Conclusion

In this thesis we have studied the dynamical behaviour of the Morse oscillator in the context of generalized coherent states. The Morse oscillator is an anharmonic oscillator that models the dynamics of many physical systems of great practical importance, for instance, diatomic molecules and polyatomic molecules. We solve the Schrödinger equation for the system to find out the eigenvectors and eigenenergies. It has been found that the Morse oscillator exhibits discrete, non degenerate and finite energy spectrum. We also derive its harmonic limit for which it reduces to the simple harmonic oscillator. The coherent states of harmonic oscillator are very well known in many areas of physics, such as quantum dynamics, quantum optics and quantum field theory. Because of their abundant application, there have been great efforts to generalize the notion of coherent states for general systems beyond the harmonic oscillator. In our work, we have studied various methods to construct generalized coherent states for anharmonic systems. In particular, we studied the methods to construct generalized coherent states suitable for the Morse oscillator. One of them is the so called Gazeau-Klauder procedure for general hamiltonian systems with discrete, non degenerate and below-bounded energy spectra.

We have constructed the generalized coherent states for the Morse oscillator based on the Gazeau-Klauder formalism and studied their basic proper-

ties. We study the time evolution of these states and analyze their temporal characteristics. We have calculated the autocorrelation function to measure the resemblance of the time evolved coherent states to the initial ones. It is shown that the Morse oscillator coherent states follow classical evolution for their short time evolution. Afterwards quantum destructive interference dominates that leads to the collapse of the states. These states undergo the process of quantum revivals and fractional revivals. Furthermore, we have constructed the time evolved coherent state wave packets both in position space and in momentum space to calculate the corresponding probability densities as a function of time. The time evolution of these probability densities results in the constructive and destructive interferences leading to the formation of quantum carpets. We have analyzed the phase space properties by means of position-momentum expectation values and Wigner quasi probability distribution function. The negativity appeared in the Wigner distribution function reflects the non classicality of the constructed coherent states of the Morse oscillator.

Bibliography

- [1] Schrödinger. E. (1926) *Naturwissenschaften* **14** 664.
- [2] Glauber. R. J. (1963) *Phys. Rev. Lett.* **10** 277.
- [3] Glauber. R. J. (1963) *Phys. Rev.* **130** 2529.
- [4] Glauber. R. J. (1963) *Phys. Rev.* **131** 2766.
- [5] Klauder. J. R. (1963) *J. Math. Phys.* **4** 1058.
- [6] Sudarshan. E. C. G. (1963) *Phys. Rev. Lett.* **10** 277.
- [7] Klauder. J. R. and McKenna. J. (1965) *J. Math. Phys.* **6** 734.
- [8] Klauder. J. R. and Sudarshan. E. C. G. (1968) *Fundamentals of Quantum Optics* (Benjamin: NewYork).
- [9] Gerry. C. C. and Knight. P.L. (2005) *Introductory Quantum Optics* (Cambridge: NewYork).
- [10] Barut. A. O. and Girardello. L. (1971) *Commun. Math. Phys.* **21** 41.
- [11] Klauder. J. R. (1996) *J. Phys. A: Math. Gen.* **29** L293.
- [12] Gazeau. J. P. and Klauder. J. R. (1999) *J. Phys. A: Math. Gen.* **32** 123.
- [13] Fox. R. F. and Choi. M. F. (2001) *Phys. Rev. A.* **64** 042104.
- [14] Fox. R. F. (1999) *Phys. Rev. A.* **51** 3241.

- [15] Perelomov. A. M. (1972) *Commun. Math. Phys.* **26** 222.
- [16] Popov. D., Dong. S. H., Pop. N., Sajfert. V. and Simon. S. (2013) *Ann. Phys.* **339** 122.
- [17] Sánchez. S. and Récamier. J. (2013) *J. Phys. A. Math. Theor.* **46** 375303.
- [18] Popov. D., Sajfert. V.,Zaharie. I. (2008) *Physica A* **387** 4459.
- [19] Antoine. J. P., Gazeau. J. P., Monceau. P., Klauder. J. R., Penson. K. A. (2001) *J. Math. Phys.* **42** 2349.
- [20] Iqbal. S., Rivière. P. and Saif. F. (2010) *Int. J. Theor. Phys.* **49** 2540.
- [21] Iqbal. S. and Saif. F. (2011) *J. Math. Phys.* **52** 082105.
- [22] Iqbal. S. and Saif. F. (2013) *J. Russ. Laser Res.* **34**, 77.
- [23] Chenaghlou. A. and Faizy. O. (2008) *J. Math. Phys.* **49** 022104.
- [24] Angelova. M. and Hussin. V. (2008) *J. Phys. A.: Math. Gen.* **41** 304016.
- [25] Morse. P. M. 1929 *Phys. Rev.* **34** 57.
- [26] Dong. S. H 2007 *Factorization Method in Quantum Mechanics* (Springer: Netherlands).
- [27] Landau. L. D. and Lifshitz. E. M. 1977 *Quantum Mechanics* (Oxford: Pergamon).
- [28] Mandel. L and Wolf. E. 1995 *Optical Coherence and Quantum Optics* (Cambridge University Press: Cambridge).
- [29] G. Herzberg. 1963 *Molecular Spectra and Molecular Structure* (Princeton: NewYork).
- [30] D. Popov 2001 *Phys. Scr.* **63** 257.

- [31] Angelova. M. and Hussin. V. 2008 *J. Phys. A: Math. Theor* **41** 304016.
- [32] Angelova. M. Hertz. A. and Hussin. V. 2012 *J. Phys. A: Math. Theor.* **45** 244007.
- [33] Jarmin. W. R. and Fraser. P. A. (1953) *II. Proc. Phys. Soc.* **66** 1153.
- [34] Vasan. V. S. and Cross. R. J. (1983) *J. Chem. Phys.* **78** 3869.
- [35] Tipping. R. H. and Ogilvie J. F. (1983) *J. Chem. Phys.* **79** 2537.
- [36] De Lima. E. F. and Hornos. J. E. M. (2005) *J. Phys. B: At. Mol. Opt. Phys.* **38** 815.
- [37] Völkel. A. R., Cuccoli. A., Spicci. M. and Tognetti. V. (1993) *Phys. Lett. A* **182** 60.
- [38] Talukdar. B., Chatterji. M. and Banerjee. P. (1979) *Pramana* **13** 15.
- [39] Lee. H. W. and Scully. M. O. (1982) *J. Chem. Phys.* **77** 4604.
- [40] Frank. A., Rivera. A. L. and Wolf. K. B. (2000) *Phys. Rev. A.* **61** 054102.
- [41] Peder Dahl. J. and Springborg. M. (1988) *J. Chem. Phys.* **88** 4535.
- [42] Carruthers and Dy. K. S 1966. *Phys. Rev.* **147** 214.
- [43] Takahashi. Y. and Shibata. F 1975 *J. Phys. Soc. Japan.* **38** 656.
- [44] Botke. J. C, Scalapino. D. J and Sugar. R. L 1974 *Phys. Rev. D* **9** 813.
- [45] Eriksson. K. E, Mukunda. N and Skagerstam. S 1981 *Phys. Rev. D* **24** 2615.
- [46] Klauder. J. R and Skagerstam. B. S 1985 *Coherent States: Applications in Physics and Mathematical Physics*(Singapore: World Scientific).

- [47] Ali. S. T, Antoine. J. P and Gazeau. J. P 2000 *Coherent States, Wavelets and Their Generalizations*(*Graduate Texts in Contemporary physics*) (New York: Springer)
- [48] Glauber. R. J. (1966) *Phys. Lett.* **21** 650.
- [49] Robinett. R. W. (2004) *Phys. Rep.* **392** 1.
- [50] Buchleitner. A. (2004) *Phys. Rep* **368** 409.
- [51] Gutschick. V.P. and Nieto. M. M. (1980) *Phys. Rev. D.* **22** 403.
- [52] Wigner. E. P. 1932 *Phys. Rev.* **40** 794.
- [53] Hudson. R. L. 1974 *Rep. Math. Phys.* **6** 249.
- [54] Tatarski. V. I. 1983 *Sov. Phys. Usp.* **26** 311.