COHERENCE CONTROL OF TUNNELING

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A THESIS APPROVED BY THE DEPARTMENT OF THEORETICAL AND
APPLIED PHYSICS

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ABSTRACT

The phase space representation of quantum mechanics are well known as powerful tools for studying the correspondence between the density operator and classical distributions in phase space. This representation, known as the third formulation of quantum mechanics, is given in terms of the joint probability distribution (or more precisely the quasi-probability), and is independent of the conventional Hilbert space or the path integral formulations. In this representation on needs not choosing-coordinate or momentum - it works in the full space, accommodating the uncertainty principle, and offering a unique insights into the classical limit of quantum theory [1].

Tunneling is a genuine quantum effect discovered long agosince the heyday of quantum mechanics. This manifests itself, for instance, as quantum particle passing through a classically forbidden barrier; the energy of the particle being smaller than that of the barrier. Although tunneling can be predicted in few simple systems, it remains a formidable task in a vast majority of quantum systems. Track Tunneling in a system maybe essential for understanding of its behavior.

In this work, we want to make use of an indicator of quantumness (or non-classicality) to control tunnelling in dynamical systems. This indicator [6], has been successfully tested in a large number of quantum states of infinite dimensional Hilbert space. It is based on the relative volume of the negative part of the Wigner function and is a quantitative measure of the degree to which a system is quantum. Attempts have been trying to link the negativity of the Wigner function with the entanglement of the analysed state on a composed Hilbert space [7].

To proceed, we will first review fundamentals of quantum mechanics in phase space focusing mainly on the role of different distribution functions. In particular, we will make use of the indicator of the Nonclassicality [6] to explore few quantum states including Fock states, Schrondinger cats, and so on. Then we will consider a tunnel model system such as ammonia (or Umbrella) for which coherent destruction of tunnelling has been revealed [8, 9]. Finally, we hope to have full control over this tunnelling model by means of that indicator [6].

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DEDICATION

I dedicate this project to my Lord and Saviour Jesus Christ, Who in His infinite mercy has used me to rewrite my family history. To my late father, Folarin Saubana Adio. I will never forget your immense sacrifice for me. I am what I am today because you stood by me. May your gentle soul rest in perfect peace (Amen).

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INTRODUCTION

1.1 Formulation of Quantum Mechanics

In this thesis, we want to use the indicator of non-classicality to control tunneling in Ammonia System (Coherence Control of Tunneling). But before we do that, we shall take our time to explore different formulations in quantum mechanics. There are at least three logically autonomous alternative paths to quantization. The first is the standard one utilizing operators in Hilbert space, developed by Heisenberg, Schrodinger, Dirac, and others in the 1920s. The second one relies on path integrals, and was conceived by Dirac[14] and constructed by Feynman. The third one (the bronze medal!) is the phase-space formulation(which is the focus of this thesis). It is based on Wigner's (1932) quasi-distribution function[12] and Weyl's (1927) correspondence[13] between ordinary c-number functions in phase space and quantummechanical operators in Hilbert space.

1.1.1 Path Integral Formulation

The path integral formulation of quantum mechanics is a description of quantum theory that generalizes the action principle of classical mechanics. It replaces the classical notion of a single, unique classical trajectory for a system with a sum, or functional integral, over an infinity of quantum-mechanically possible trajectories to compute a quantum amplitude.This formulation has proven crucial to the subsequent development of theoretical physics, because manifest Lorentz covariance (time and space components of quantities enter equations in the same way) is easier to achieve than in the operator formalism of canonical quantization. Unlike previous methods, the path integral allows a physicist to easily change coordinates between very different canonical descriptions of the same quantum system. Another advantage is that it is in practice easier to guess the correct form of the Lagrangian of a theory, which naturally enters the path integrals (for interactions of a certain type, these are coordinate space or Feynman path integrals), than the Hamiltonian. Pos-

sible downsides of the approach include that unitarity (this is related to conservation of probability; the probabilities of all physically possible outcomes must add up to one) of the S-matrix is obscure in the formulation. The path-integral approach has been proved to be equivalent to the other formalisms of quantum mechanics and quantum field theory. Thus, by deriving either approach from the other, problems associated with one or the other approach (as exemplified by Lorentz covariance or unitarity) go away [10]. Path integrals are used in a variety of fields, including stochastic dynamics, polymer physics, protein folding, field theories, quantum mechanics, quantum field theories, quantum gravity and string theory. The basic idea is to sum up all contributing paths.
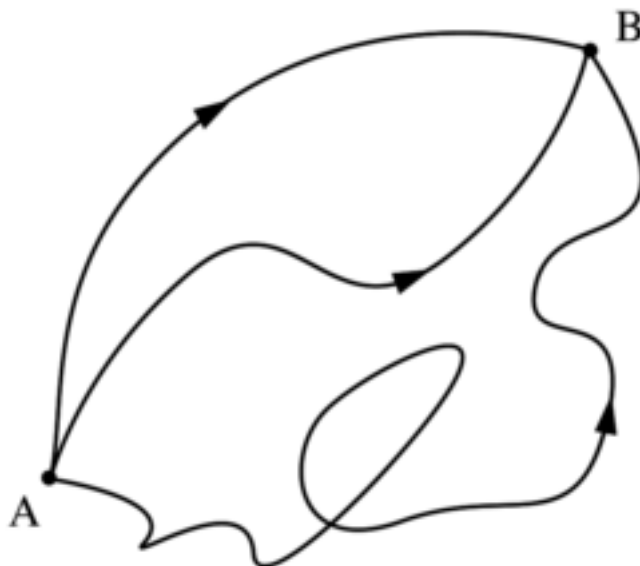

Figure 1.1: Path Integral Formulation

The path integral formula in terms of the wave function is given as

$$\psi(x, t) = \frac{1}{Z} \int_{x(0)=x} \mathcal{D}\mathbf{x} e^{iS[\mathbf{x}, \dot{\mathbf{x}}]} \psi_0(\mathbf{x}(t)) \tag{1.1}$$

where $\mathcal{D}\mathbf{x}$ denotes integration over all paths $\mathbf{x}$ with $\mathbf{x}(0) = x$ and where Z is a normalization factor. Here S is the action, given by $S[\mathbf{x}, \dot{\mathbf{x}}] = \int dt \, L(\mathbf{x}(t), \dot{\mathbf{x}}(t))$

1.1.2 Hilbert Space Formulation

The mathematical formulations of quantum mechanics are those mathematical formalisms that permit a rigorous description of quantum mechanics. Such are distinguished from mathematical formalisms for theories developed prior to the early 1900s

by the use of abstract mathematical structures, such as infinite-dimensional Hilbert spaces and operators on these spaces. Many of these structures are drawn from functional analysis, a research area within pure mathematics that was influenced in part by the needs of quantum mechanics. In brief, values of physical observables such as energy and momentum were no longer considered as values of functions on phase space, but as eigenvalues; more precisely as spectral values of linear operators in Hilbert space [11]. These formulations of quantum mechanics continue to be used today. At the heart of the description are ideas of quantum state and quantum observables which are radically different from those used in previous models of physical reality. While the mathematics permits calculation of many quantities that can be measured experimentally, there is a definite theoretical limit to values that can be simultaneously measured. This limitation was first elucidated by Heisenberg through a thought experiment, and is represented mathematically in the new formalism by the non-commutativity of operators representing quantum observables.

1.1.3 The Phase Space Formulation

Phase Space formulation of quantum mechanics The phase-space formulation of quantum mechanics places the position and momentum variables on equal footing, in phase space. The two key features of the phase-space formulation are that the quantum state is described by a quasi-probability distribution (instead of a wave function, state vector, or density matrix) and operator multiplication is replaced by a star product. Wigner's quasi-probability distribution function in phase-space is a special (Weyl– Wigner) representation of the density matrix. It has been useful in describing transport in quantum optics, nuclear physics, quantum computing, decoherence, and chaos. It is also of importance in signal processing, and the mathematics of algebraic deformation. A remarkable aspect of its internal logic, pioneered by Groenewold and Moyal, has only emerged in the last quarter-century: It furnishes a third, alternative, formulation of quantum mechanics, independent of the conventional Hilbert space or path integral formulations. In this logically complete and self-standing formulation, one need not choose sides between coordinate or momentum space. It works in full phase-space, accommodating the uncertainty principle; and it offers unique insights into the classical limit of quantum theory: The variables (observables) in this formulation are c-number functions in phase space instead of operators, with the same interpretation as their classical counterparts, but are composed together in novel algebraic ways. A variety of these representation exist,

including Wigner [12], Husimi [3], P [4], Huwi [5], and are distinct one to another by the way they highlight classical structures against a background of quantum interferences. This complete formulation is based on the Wigner function (WF), which is a quasiprobability distribution function in phase-space,

$$f(x,p) = \frac{1}{2\pi} \int dy \psi^* \left(x - \frac{\hbar}{2}y \right) e^{-iyp} \psi \left(x + \frac{\hbar}{2}y \right) \tag{1.2}$$

It is a generating function for all spatial autocorrelation functions of a given quantummechanical wave-function $\psi(x)$. More importantly, it is a special representation of the density matrix (in the Weyl correspondence, as detailed in chapter 2)

1.2   Coherent State

Coherent states play an important role in quantum optics, especially in laser physics and much work was performed in this field by Roy J. Glauber who was awarded the 2005 Nobel prize for his contribution to the quantum theory of optical coherence.The state describing a laser beam can be briefly characterized by (i) an indefinite number of photons, (ii) A precisely defined phase,

in contrast to a state with fixed particle number, where the phase is completely random. There also exists an uncertainty relation describing this contrast. It can be formulated for the uncertainties of amplitude and phase of the state, where the inequality reaches a minimum for coherent states [16]

$$\Delta N \Delta(sin\Phi) \geq \frac{1}{2} cos(\Phi) \tag{1.3}$$

which, for small Φ, reduces to

$$\Delta N \Delta(\Phi) \geq \frac{1}{2} \tag{1.4}$$

1.2.1   Definition and Properties of Coherent States

A coherent state $|\alpha\rangle$, also called Glauber state, is defined as eigenstate of the amplitude operator which is the annihilation operator a , with eigenvalues $\alpha \in \mathbb{C}$

$$a |\alpha\rangle = \alpha |\alpha\rangle$$

Since a is a non-hermitian operator the phase $\alpha = |\alpha|e^{i\varphi} \in \mathbb{C}$ is a complex number and corresponds to the complex wave amplitude in classical optics. Thus coherent states are wave-like states of the electromagnetic oscillator.

Properties of Coherent States

1. A vacuum $|0\rangle$ is a coherent state with $\alpha = 0$

2. mean energy of the Harmonic Oscillator can be obtained between the coherent states

$$\langle H \rangle = \langle \alpha | H | \alpha \rangle = \langle \alpha | (a^+ a + \frac{1}{2}) | \alpha \rangle = \hbar\omega(|\alpha|^2 + \frac{1}{2}) \tag{1.5}$$

where $\hbar\omega|\alpha|^2$ is the classical wave intensity

1.2.2 Density Matrix or Density Operator

A density matrix or density operator is a matrix that describes the statistical state of a system in quantum mechanics. The density matrix is especially helpful for dealing with mixed states, which consist of a statistical ensemble of several different quantum systems. The opposite of a mixed state is a pure state.

The density matrix is formally defined as the outer product of the wavefunction and its conjugate.

$$\rho(t) \equiv |\psi(t)\rangle \langle\psi(t)| \tag{1.6}$$

This implies that if you specify a state $|\chi\rangle$, the integral $\langle\chi| \rho |\chi\rangle$ gives the probability of finding a particle in the state $|\chi\rangle$ Its name derives from the observation that it plays the quantum role of a probability density. If we think of the statistical description of a classical observable obtained from moments of a probability distribution P, then ρ plays the role of P in the quantum case:

$$\langle A \rangle = \int AP(A)dA \tag{1.7a}$$

$$\langle A \rangle = \langle\psi| A |\psi\rangle = Tr[A\rho] \tag{1.7b}$$

where $Tr[A\rho]$ refers to tracing over the diagonal elements of the matrix. The question is that why do we need a density matrix? We need a density matrix because It is a practical tool when dealing with mixed states.Pure states are those that are characterized by a single wavefunction. Mixed states refer to statistical mixtures in which we have imperfect information about the system, for which me must perform statistical averages in order to describe quantum observables. A mixed state refers to any case in which we subdivide a microscopic or macroscopic system into an ensemble, for which there is initially no phase relationship between the elements of the mixture. Examples include an ensemble at thermal equilibrium, and independently prepared states[15].

Properties of Density Matrix

1. ρ is hermitian: $\rho^*_{nm} = \rho_{nm}$

2. Normalization: $Tr[\rho] = 1$

3. $Tr(\rho^2) = 1$ for pure state

4. $Tr(\rho^2) \leq 1$ for mixed state

1.3 Dynamical Tunneling

Tunneling has remained a special phenomenon, a quintessential quantum effect, starting with the early days of quantum theory. Nearly a century's worth of theoretical and experimental studies have highlighted the crucial role of tunneling in various physical phenomenal. The far-reaching implications of tunneling are evident in diverse fields including nuclear, atomic, molecular physics, and more recently, in the area of mesoscopic science. Despite the obvious relevance of this topic to a wide range of disciplines, an interdisciplinary scientific community devoted to tunneling has not yet developed to a satisfactory degree. One may attribute this, at first glance, to the apparent simplicity of a generic tunneling process, which basically involves **only a quantum particle that crosses a classical barrier** due to the evanescent components of its wave function. The quantitative description of this seemingly simple process, however, can become rather intricate and rich if more than one particle and/or more than one spatial dimension are effectively involved. This is especially the case for "**dynamical Tunneling**," which essentially denotes classically forbidden transitions through dynamical rather than energetic barriers, that is barriers that are formed by constraints of the underlying classical dynamics related to exact or approximate constants of motion[17].

1.3.1 Tunnel Model System(Ammonia or Umbrella)

The ammonia molecule helps illustrate how to simplify the description of a complicated problem. In an ammonia molecule, atoms located at the vertices of a pyramid; three hydrogen atoms in a plane and a nitrogen atom above or below that plane. The description of this molecule can be complicated because it is possible to have an infinite number of motion states, namely,rotation around any axis, translational motion in any direction and vibrational motions[18].
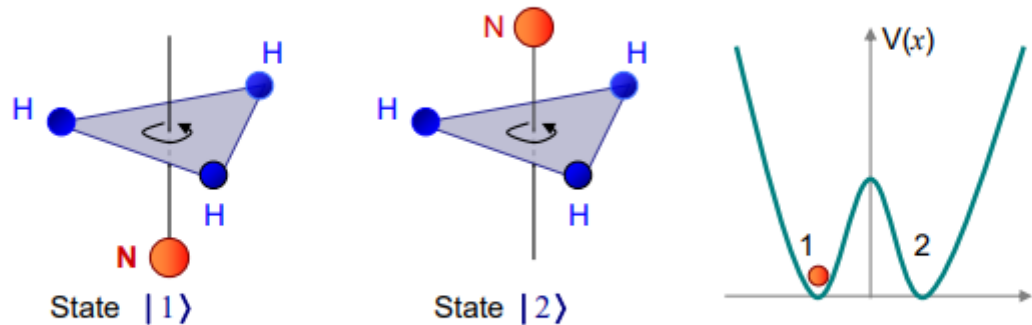
Fig. 2 Spatial configuration of states $|1\rangle$ and $|2\rangle$ for the NH_3 molecule. The curve on the right shows the potential energy of the N atom as a function of the distance from the plane containing the hydrogen atoms.

The molecule has two possible positions for the nitrogen atom (as shown in the figure above), which define the two base states $|1\rangle$ and $|2\rangle$. Where state $|1\rangle$ defines the "down" state of the molecule (a given charge distribution corresponding to the case when the nitrogen is below the plane defined by the three hydrogen atoms.) and state $|2\rangle$ defines the "up" state of the molecule (a given charge distribution corresponding to the case when the nitrogen is above the plane defined by the three hydrogen atoms.)

1.4 The Wigner Function

Because there is no uncertainty principle in classical physics, it is possible to know a particle's momentum and position at the same time to an arbitrary precision. Quantum mechanics is a fundamental theory in physics which describes nature at the smallest scales of energy levels of atoms and subatomic particles [19]. Quantum mechanics differs from classical physics in that energy, momentum, angular momentum and other quantities of a bound system are restricted to discrete values (quantization); objects have characteristics of both particles and waves (wave-particle duality); and there are limits to the precision with which quantities can be measured (uncertainty principle). This uncertainty principle makes it possible to know both position (x) and momentum (p) at the same time. In the standard formulation of quantum mechanics one works with probability densities instead. One for the wave-function in position-basis and one for the wave-function in the momentum

basis.

$$P(x) = |\psi(x)|^2$$

$$P(x) = |\phi(k)|^2$$

Where the two functions are connected by a Fourier transform and use $p = \hbar k$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)e^{-ikx}dx$$

It would be desirable to have a single function that could display the probability in both position and momentum simultaneously. The Wigner function is a function constructed to do just that. It must also be able to give the correct expectation values for operators. What one desire is to have a probability distribution in phase space P(x,p), that is positive everywhere and such that

$$\left\langle \hat{A} \right\rangle = \iint P(x,p)A(x,p)dxdp \tag{1.8}$$

This gives the expectation value of the operator A(x,p). It should be noted that because of Heisenberg's uncertainty principle, it is not possible to find such a probability distribution. The Wigner function comes close to fulfil these demand but it will not have a direct physical interpretation as a probability distribution we know from classical physics. For example, the Wigner function can be negative in regions of phase space, which have no physical meaning if one thinks of it as a probability distribution. Therefore the Wigner function is quasi-distribution. A main goal of quantum mechanics is to obtain expectation values for physical observables. If the Wigner function is to be a complete formulation of quantum mechanics, it must also be able to reproduce the expectation values of all functions of x and p. When using the Wigner function, the expectation values are obtained in conjunction with the closely associated Weyl transforms of the operators corresponding to physical observables. The correct Weyl-transform is critical for obtaining the spread of the energy of a state; without it, the Wigner function is little more than a visual aid for understanding quantum states.

1.4.1 The Weyl Transform and the Wigner Function

In order to construct a Wigner function, what we mean to do is to construct a new formalism of quantum mechanics based on a phase space formalism. To create such a formalism successfully, one needs a mapping between functions in the quantum

phase space formulation and Hilbert space operators in the Schrodinger picture. This mapping is given by the Weyl-transform $\tilde{A}$ of an operator $\hat{A}$ defined in the following way

$$\tilde{A}(x,p) = \int e^{-\frac{ipy}{\hbar}} \left\langle x + \frac{y}{2}|\hat{A}|x - \frac{y}{2} \right\rangle dy \tag{1.9}$$

Where the operator has been expressed in the x basis as the matrix $\langle x'|\hat{A}|x\rangle$. The Weyl transform will be indicated by tilde. The Weyl transform converts an operator into a function of x and p. The Weyl transform can also be expressed in terms of matrix elements of the operator in the momentum basis,

$$\tilde{A}(x,p) = \int e^{\frac{ixu}{\hbar}} \left\langle p + \frac{u}{2}|\hat{A}|p - \frac{u}{2} \right\rangle dy \tag{1.10}$$

A key property of the Weyl transform is that the trace of the product of two operators $\hat{A}$ and $\hat{B}$ is given by the integral over phase space of the product of their Weyl transforms,

$$Tr[\hat{A}\hat{B}] = \frac{1}{h} \iint \tilde{A}(x,p)\tilde{B}(x,p)dxdp \tag{1.11}$$

The prove of equation(2.4) is in appendix A of this Thesis. To represent the state, we make use of the density operator $\hat{\rho}$. For a pure state $|\psi\rangle$ it is given by $\hat{\rho} = |\psi\rangle\langle\psi|$. Which is expressed in the position basis as $\langle x|\hat{\rho}|x'\rangle = \psi(x)\psi^*(x')$. One of the virtues of the density operator and thus the Wigner function is that it is easily generalized to mixed states. If we form the trace of $\hat{p}$ with the operator corresponding to the observable A, we have for the expectation value

$$Tr[\hat{\rho}\hat{A}] = Tr[|\psi\rangle\langle\psi|\hat{A}] = \langle\psi|\hat{A}|\psi\rangle = \langle A\rangle \tag{1.12}$$

Thus using equation (2.4) we have

$$\langle A\rangle = Tr[\hat{\rho}\hat{A}] = \frac{1}{h}\int \tilde{\rho}\tilde{A}dxdp \tag{1.13}$$

The Wigner function is thus defined as

$$W(x,p) = \tilde{\rho}/h = \frac{1}{h}\int e^{-\frac{ipy}{\hbar}} \psi(x + y/2)\psi^*(x - y/2)dy \tag{1.14}$$

And the expectation value of A is given by

$$\langle A\rangle = \iint W(x,p)\tilde{A}(x,p)dxdp \tag{1.15}$$

We can vividly see that the expectation value of A has been obtained by what looks like the average of the physical quantity represented by $\tilde{A}(x,p)$ over phase space

with probability density W(x,p) characterizing the state. If the Wigner function is integrated over p alone and use is made of $\int e^{\frac{ipx}{\hbar}} dp = h\delta(x)$, we have

$$\int W(x,p)dp = \psi^*(x)\psi(x) \tag{1.16}$$

Equation (2.9) gives the probability distribution for x. A similar integral over x gives

$$\int W(x,p)dx = \varphi^*(p)\varphi(p) \tag{1.17}$$

Equation (2.10) gives the probability distribution for the momentum variable. Thus, the Wigner function represents the distribution in phase space represented by $\psi(x)$. The projection of W(x,p) onto the x axis gives the probability distribution in x, and the projection on the ρ axis gives the distribution in p. Expectation values of physical quantities are obtained by averaging $\tilde{A}(x,p)$ over phase space. We shall see that the interpretation of W(x,p) as a simple probability distribution is spoiled by a number of features.

1.4.2   Characteristics Of The Weyl And Wigner Function

A direct consequence of the definition of the Wigner function in equation (2.7) is that it is real as can be seen by taking the complex conjugate of equation (2.7) and changing the variable of integration from y to –y. that is,

$$W(x,p) = \tilde{\rho}/h = \frac{1}{h}\int e^{-\frac{ipy}{\hbar}}\psi(x + y/2)\psi^*(x - y/2)dy$$

$$W(x,p)^* = \tilde{\rho}/h = \frac{1}{h}\int e^{-\frac{ipy}{\hbar}}\psi^*(x - y/2)\psi(x + y/2)dy \tag{1.18}$$

Using equation (2.3) one can express the Wigner function in terms of the momentum representation of $|\psi\rangle$

$$W(x,p) = \tilde{\rho}/h = \frac{1}{h}\int e^{\frac{ixu}{\hbar}}\langle p + u/2|\psi\rangle\langle\psi|p - u/2\rangle \tag{1.19a}$$

$$W(x,p) = \tilde{\rho}/h = \frac{1}{h}\int e^{\frac{ixu}{\hbar}}\varphi^*(p + u/2)\varphi(p - u/2)du \tag{1.19b}$$

The Weyl transform of the identity operator $\hat{I}$ is I because

$$\tilde{I} = \int e^{-\frac{ipy}{\hbar}}\left\langle x + \frac{y}{2}\Big|\hat{I}\Big|x - \frac{y}{2}\right\rangle dy = \int e^{-\frac{ipy}{\hbar}}\delta(x + \frac{y}{2} - (x - \frac{y}{2}))dy = 1 \tag{1.20}$$

A feature of the Wigner function is that it is normalized in x,p space. This is easily seen by the following

$$\iint W(x,p)\tilde{I} = \iint W(x,p)dxdp = Tr[\hat{\rho}] = 1 \qquad (1.21)$$

Thus $W(x,p)$ is normalized in x,p space. Also from the definition of the density operator we can vividly see that for pure state $\hat{\rho}^2 = \hat{\rho}$, and thus $Tr[\hat{\rho}^2] = Tr[\hat{\rho}] = 1$. We can infer from this relation and equations (2.4) and (2.7) that

$$\iint W(x,p)^2 dxdp = \frac{1}{h} \qquad (1.22)$$

It should be noted that the Wigner functions have a reasonable **translation property**. Meaning that if the wave function $\psi(x)$ gives the Wigner function $W(x,p)$, then the wave function $\psi(x-d)$ will give $W(x-d,p)$. This shows that a shifts in the wave function lead to a corresponding shifts in the Wigner function in the position variable x. In the same vein, if the original wave function is replaced with $\psi(x)e^{\frac{ixd_p}{\hbar}}$, the new Wigner function becomes $W(x,p-d_p)$. This vividly shows that a shift in momentum of the original wave function lead to a corresponding shifts of the Wigner function in the momentum variable p. Both of these properties follow directly from the definition of the Wigner function we defined earlier in equation(1.7). The signs in these shifts might be a little disturbing. If $\psi(x)$ is concentrated about x_o, then $\psi(x-d)$ will be concentrated about $x_o + d$. In addition, if the $\psi(x)$ has a certain momentum distribution, then $\psi(x)e^{\frac{ixd_p}{\hbar}}$ will have the same distribution shifted by $+d_p$. This means that each of the shifts correspondingly shift their respective distribution by $+d$ or $+d_p$, respectively. Now, given two density operators $\hat{\rho}_a$ and $\hat{\rho}_b$, from different states ψ_a and ψ_b respectively. forming the combination of this gives

$$Tr[\hat{\rho}_a\hat{\rho}_b] = |\langle\psi_a|\psi_b\rangle|^2 \qquad (1.23)$$

The Weyl transform of Equation(2.16) using equation(2.4) and (2.7)

$$\iint W_a(x,p)W_b(x,p)dxdp = \frac{1}{h}|\langle\psi_a|\psi_b\rangle|^2 \qquad (1.24)$$

This shows that the product of Wigner functions integrated over phase space is the square of the inner product of the original wave functions divided by h. The left-hand side of equation(2.17) acts as a positive inner product of the original states. If we consider orthogonal states where $\langle\psi_a|\psi_b\rangle = 0$

$$\iint W_a(x,p)W_b(x,p)dxdp = 0 \qquad (1.25)$$

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This can only be true if and only if the Wigner function is negative in the region of phase space. This is very different from the classical case and shows us that the Wigner function does not represent a physical property. The integral of the Wigner function over x and p is the only one that has physical meaning. We cannot not think of the Wigner function the same way we think of a classical distribution but we can think of it as a mathematical object that will help us to calculate physical observables in just the same way we think of the wavefunction in the Schrödinger picture.

Another key property of a Wigner function is that it must fulfill $|W(x,p)| \leq \frac{1}{\pi\hbar}$. This follows from the fact that we can rewrite the definition of the Wigner function in equation(2.7) as a product of two wave functions as shown

$$W(x,p) = \frac{1}{\pi\hbar} \int dy \psi_1(y)\psi_2^*(y) \tag{1.26}$$

where we have defined the following normalized wave functions $\psi_1(y) = e^{-\frac{ipy}{\hbar}} \frac{\psi(x+\frac{y}{2})}{\sqrt{2}}$ and $\psi_2(y) = \frac{\psi(x-\frac{y}{2})}{\sqrt{2}}$ and use the relation

$$\int \psi(x - \frac{y}{2})\psi^*(x - \frac{y}{2})dy = 2\int \psi(x - \frac{y}{2})\psi^*(x - \frac{y}{2})d(\frac{y}{2}) = 2 \tag{1.27}$$

From the definition of the Wigner function in equation (2.7), it is clear that an even wavefunction at $0,0$ will have a Wigner function that takes on the value $+\frac{1}{\pi\hbar}$. An odd wavefunction will then have a Wigner function at $0,0$ with the value $-\frac{1}{\pi\hbar}$.

The expectation value is obtained through the average of a physical quantity represented by $\tilde{A}(x,p)$ over phase space with quasi-probability density $W(x,p)$ characterizing the state.The expectation values of the position x and momentum p are now given by

$$\langle x \rangle = \iint W(x,p)x dx dp \tag{1.28a}$$

$$\langle p \rangle = \iint W(x,p)p dx dp \tag{1.28b}$$

We can now categorically generalize this that to find the expectation value of an operator from the Wigner function, one has to consider the Weyl-transform of the said operator. If we have an operator $\hat{A}(x)$ that depends solely on $\hat{x}$ which allows us to write $\hat{A} = A(\hat{x})$. The Weyl-transform for an operator of this form is easy. From equations(2.2) we have

$$\tilde{A} = \int e^{-\frac{ipy}{\hbar}} \left\langle x + \frac{y}{2}|\hat{A}(\hat{x})|x - \frac{y}{2} \right\rangle dy = \int e^{-\frac{ipy}{\hbar}} A\left(x - \frac{y}{2}\right)\delta y = A(x) \tag{1.29}$$

This shows that the Weyl-transform of such an operator is simply a function A with the operator $\hat{x}$ replaced with x. It is the same for an operator $\hat{A}(\hat{p})$ since the Weyl-transform can be defined in a momentum representation instead of a position representation [20].Therefore, for an operator $\hat{B}(\hat{p})$ that depends only on $\hat{p}$ the Weyl-transform is the function of $B(p)$. This extends to sums of operators that only depends on $\tilde{x}$ and $\hat{p}$. Considering a Hamiltonian operator $\hat{H}(\hat{x}, \hat{p}) = \hat{T}(\hat{p}) + \hat{U}(\hat{x})$. This operator will have the Weyl transform $H(x, p) = T(p) + U(x)$. So from this result, we can determine the expectation value from this Hamiltonian operator. The expectation value of T, U and H are given by

$$\langle T \rangle = \iint dx dp W(x, p) T(p) \tag{1.30a}$$

$$\langle U \rangle = \iint dx dp W(x, p) U(x) \tag{1.30b}$$

$$\langle H \rangle = \iint dx dp W(x, p) H(x, p) \tag{1.30c}$$

1.5 Time Evolution of the Wigner Function

For a stationary state we have the solution as

$$\psi_n(x, t) = u_n(x) e^{-\frac{i E_n t}{\hbar}} \tag{1.31}$$

where $u_n(x)$ is a real function.By looking at definition (2.7), we can clearly see that for a stationary state, the Wigner function does not explicitly depend on time. The phases containing the time evolution $e^{-\frac{iEt}{\hbar}}$ will always cancel out.

It is however possible possible to derive an equation that governs the time evolution of the Wigner function. This approaches uses the fact that x and p will depend on time t. To describe the time evolution of a given Wigner function, we simply take the derivative with respect to time t and use the Schrödinger equation to eliminate the partial derivative of the wavefunction.

$$\frac{\partial W}{\partial t} = \frac{1}{2\pi\hbar} \int dy e^{-\frac{ipy}{\hbar}} \left\{ \frac{\partial \psi^*(x - \frac{y}{2})}{\partial t} \psi\left(x + \frac{y}{2}\right) + \frac{\partial \psi(x + \frac{y}{2})}{\partial t} \psi^*\left(x - \frac{y}{2}\right) \right\} \tag{1.32}$$

$$\frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar}{2im} \frac{\partial^2 \psi(x, t)}{\partial x^2} + \frac{1}{i\hbar} U(x) \psi(x, t) \tag{1.33}$$

by substituting equation(2.26) into (2.25), we obtain

$$\frac{\partial W}{\partial t} = \frac{1}{2\pi\hbar} \int dy e^{-\frac{ipy}{\hbar}} \left\{ \frac{\hbar}{2im} \frac{\partial^2 \psi(x,t)}{\partial x^2} \psi\left(x + \frac{y}{2}\right) - \frac{1}{i\hbar} U\left(x - \frac{y}{2}\right) \psi^*\left(x - \frac{y}{2}\right) \psi\left(x + \frac{y}{2}\right) \right.$$
$$\left. - \frac{\hbar}{2im} \frac{\partial^2 \psi(x + \frac{y}{2})}{\partial x^2} \psi^*\left(x - \frac{y}{2}\right) + \frac{1}{i\hbar} U\left(x + \frac{y}{2}\right) \psi\left(x + \frac{y}{2}\right) \psi^*\left(x - \frac{y}{2}\right) \right\}$$

$$(1.34)$$

Equation(1.27) can be written as

$$\frac{\partial W}{\partial t} = \frac{1}{4\pi im} \int dy e^{-\frac{ipy}{\hbar}} \left\{ \frac{\partial^2 \psi^*(x - \frac{y}{2})}{\partial x^2} \psi\left(x + \frac{y}{2}\right) - \frac{\partial^2 \psi(x + \frac{y}{2})}{\partial x^2} \psi^*\left(x - \frac{y}{2}\right) \right\}$$
$$+ \frac{2\pi}{i\hbar^2} \int dy e^{-\frac{ipy}{\hbar}} \left\{ U\left(x + \frac{y}{2}\right) - U\left(x - \frac{y}{2}\right) \right\} \psi\left(x + \frac{y}{2}\right) \psi^*\left(x - \frac{y}{2}\right)$$

$$(1.35)$$

This defines

$$\frac{\partial W}{\partial t} = \frac{\partial W_T}{\partial t} + \frac{\partial W_U}{\partial t} \qquad (1.36)$$

where

$$\frac{\partial W_T}{\partial t} = \frac{1}{4\pi im} \int dy e^{-\frac{ipy}{\hbar}} \left\{ \frac{\partial^2 \psi^*(x - \frac{y}{2})}{\partial x^2} \psi\left(x + \frac{y}{2}\right) - \frac{\partial^2 \psi(x + \frac{y}{2})}{\partial x^2} \psi^*\left(x - \frac{y}{2}\right) \right\}$$

$$(1.37)$$

and

$$\frac{\partial W_U}{\partial t} = \frac{2\pi}{i\hbar^2} \int dy e^{-\frac{ipy}{\hbar}} \left\{ U\left(x + \frac{y}{2}\right) - U\left(x - \frac{y}{2}\right) \right\} \psi\left(x + \frac{y}{2}\right) \psi^*\left(x - \frac{y}{2}\right) \quad (1.38)$$

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CHAPTER 2

THEORETICAL BACKGROUND

As aforementioned in the introduction, We want to use the indicator of non-classicality which was pioneered by Kenfack [6] to explore few quantum states such as Schrödinger cats state, Fock states and so on. In this project, I used the same indicator of quantumness to control tunneling in Ammonia or umbrella system (i.e Coherence Control of Tunneling) in which Coherence Destruction of Tunneling has been achieved by grossmann [9, 8]. To proceed, we start by analysing pure quantum states in an infinite dimensional Hilbert space which is useful to distinguish a family of coherent states, localized in the classical phase space and minimizing the uncertainty principle. These quantum analogues of points in the classical phase space are often considered as 'classical' states. For an arbitrary quantum state one may ask or pose a natural question, to what extent is it 'non-classical' in a sense that its properties differ from that of coherent states? In other words, is there any parameter that may categorically reflect the degree of non-classicality of a given quantum state? This question was motivated by the first observation of non-classical features of electromagnetic fields such as sub-Poissonian statistics, antibunching and squeezing. In addition, it is well known that the interaction of linear or non-linear devices with quantum states may cause them to flip from one state to another; for example, nonlinear devices may produce non-classical states from their interaction with the vacuum or a classical field. A systematic survey of non-classical properties of quantum states would be worthwhile because of the current ever increasing number of experiments in nonlinear optics. An earlier attempt to shed some light on the non-classicality of a quantum state was pioneered by Mandel [22], who investigated radiation fields and introduced a parameter q to measure the deviation of the photon number statistics from the Poissonian distribution, characteristic of coherent states.

In general, to define a measure of non-classicality of quantum states one can follow several different approaches [23]. Distinguishing a certain set C of states (e.g. the set of coherent states $|\psi\rangle$), one looks for the distance of an analysed pure state $|\psi\rangle$ to this set, by minimizing a distance $d(|\psi\rangle, |\psi\rangle)$ over the entire set C. Such a

scheme based on the trace distance was first used by Hillery [59, 25], while other distances (the Hilbert– Schmidt distance [26, 27] or the Bures distance [28, 29]) were later used for this purpose. The same approach is also applicable to characterize mixed quantum states: minimizing the distance of the density ρ to the set of coherent states is related [27, 30] to the search for the maximal fidelity (the Hilbert–Schmidt fidelity ($Tr(\rho\sigma)$ or the Bures–Uhlmann fidelity ($Tr\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$) with respect to any coherent state, $\sigma = |\sigma\rangle\langle\sigma|$. On the same footing, the Monge distance introduced in [32, 31] may be applied to describe to what extent a given mixed state is close to the manifold of coherent states.

Yet another way of proceeding is based on the generalized (Cahill) phase space representation R_τ of a pure state, which interpolates between the Husimi (Q), the Wigner (W) and the Glauber–Sudarshan (P) representations. The Cahill parameter τ is proportional to the variance of a Gaussian function one needs to convolute with P representation to obtain R_τ [33]. In particular for $\tau = 1, \frac{1}{2}, 0$ one obtains the Q-, W and P-representations, respectively. By construction the Q representation is non-negative for all states, while the Wigner function may also admit negative values, and the P representation may be singular or may not exist. The smoothing effect of R_τ is enhanced as τ increases. If τ is large enough so that R_τ becomes a positive definite regular function, thus acceptable as a classical distribution function, then the smoothing is said to be complete. The greatest lower bound τm for the critical value was adopted by Lee [34, 35], as the non-classical depth of a quantum state, and this approach was further developed in [36, 38]. The limiting value, $\tau m = 1$, corresponds to the Q function which is always acceptable as a classical distribution function. The lowest value, $\tau m = 0$, is ascribed to an arbitrary coherent state because its P function is a Dirac delta function, so its ϵ-smoothing becomes regular. The range of τm is thus $\tau m \in [0, 1]$. If the Husimi function of a pure state admits at least one zero $Q(\alpha_o) = 0$, then a Cahill R_τ distribution with a narrower smearing, $\tau < 1$, becomes negative in the vicinity of α_o. Therefore the classical depth for such quantum states is maximal, $\tau m = 1$ [36]. The only class of states for which Q representation has no zeros are the squeezed coherent states for which τm is a function of the squeezing parameter s. In the limiting case s = 0 one obtains the standard coherent state for which the $R_o = P$ distribution is a Dirac delta function, that is $\tau m = 0$. A possible way to distinguish a classical state is to require that its P-representation exists and is everywhere non-negative. Such an approach was advocated in [40] and further explored in [41], while a recent work [42] establishes a

link between the task of classifying all states with positive P-representation and the 17th Hilbert problem concerning positive polynomials. A closely related approach to characterizing quantum states is based on properties of their Wigner functions in phase space p, q. One can prove that the Wigner function is bounded from below and from above [33]. In the normalization $\iint W(q,p)dqdp = 1$ used later in this work, such a bound reads $|W(q,p)| \leq \frac{1}{\pi\hbar}$. Further bounds on integrals of the Wigner function were derived in [43], while an entropy approach to the Wigner function was developed in [44, 45]. In order to interpret the Wigner function as a classical probability distribution one needs to require that W is nonnegative. As found by Hudson in 1974 [46], this is the case for coherent or squeezed vacuum states only. A possible measure of non-classicality may thus be based on the negativity of the Wigner function which may be interpreted as a signature of quantumness. The negativity of the Wigner function has been linked to non-locality, according to the Bell inequality [47], while investigating the original Einstein–Podolsky–Rosen (EPR) state [48]. In fact Bell argued that the EPR state will not exhibit non-local effects because its Wigner function is everywhere positive, and as such will allow for a hidden variable description of correlations. However, it is now demonstrated [49, 50] that the Wigner function of the EPR state, though positive definite, provides direct evidence of nonlocality. This violation of Bell's inequality holds true for the regularized EPR state [51] and also for a correlated two-mode quantum state of light [53]. It is also worth recalling that the Wigner function can be measured experimentally [54], including the measurements of its negative values [55]. The interest put on such experiments has triggered a search for operational definitions of the Wigner functions, based on experimental setup [56, 57].

2.1   Schrödinger cat state

Schrödinger's cat is a seemingly paradoxical thought experiment devised by Erwin Schrödinger that attempts to illustrate the incompleteness of an early interpretation of quantum mechanics when going from subatomic to macroscopic systems. Schrödinger proposed his "cat" after debates with Albert Einstein over the Copenhagen interpretation, which Schrödinger defended, stating in essence that if a scenario existed where a cat could be so isolated from external interference (decoherence), the state of the cat can only be known as a superposition (combination) of possible rest states (eigenstates), because finding out (measuring the state) cannot

be done without the observer interfering with the experiment — the measurement system (the observer) is entangled with the experiment.

The thought experiment serves to illustrate the strangeness of quantum mechanics and the mathematics necessary to describe quantum states.
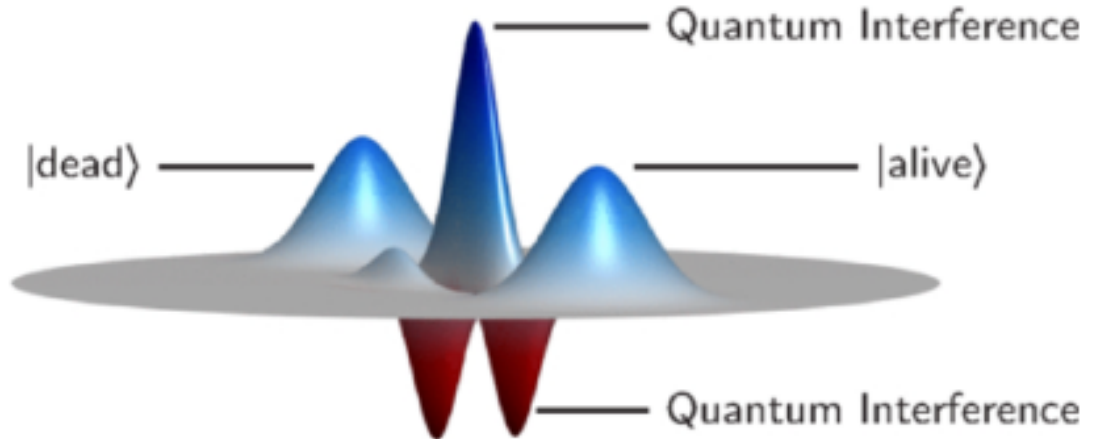

Figure 2.1: Schrodinger Cat State

The idea of a particle existing in a superposition of possible states, while a fact of quantum mechanics, is a concept that does not scale to large systems (like cats), which are not indeterminably probabilistic in nature.

Philosophically, these positions which emphasize either probability or determined outcomes are called (respectively) positivism and determinism.

2.2 Indicator Of Non-classicality

The Wigner function of a state $|\psi\rangle$ defined by

$$W_\psi(q,p) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \left\langle q - \frac{x}{2} \middle| \psi \right\rangle \left\langle \psi \middle| q + \frac{x}{2} \right\rangle \exp(ipx) \qquad (2.1)$$

satisfies the normalization condition $\iint W_\psi(q,p)dpdq = 1$. Hence the double volume of the integrated negative part of the wigner function may be written as

$$\delta(\psi) = \iint \left[| W_\psi(q,p) | - W_\psi(q,p) \right] dpdq = \iint | W_\psi(q,p) | \, dqdp - 1 \qquad (2.2)$$

By definition, the quantity δ is equal to zero for coherent and squeezed vacuum states, for which W is non-negative. equation(2.2) is the indicator of non-classicality which always measures the degree to which a system is quantum. As we can vividly see that by giving a Wigner function, we can perform double integration over its absolute function minus one to get the degree at which that system is quantum. It is also worth noting that for a vacuum, the indicator gives zero. In the case of Kenfack [6] (The pioneer of this indicator), he used it to measure the quantumness of a system by exploring different quantum system as mentioned earlier but in this work, I want to use the same indicator of quantumness to control tunneling in ammonia system[9]. As we shall see later, by giving a Hamiltonian that describe an ammonia system, one can easily get the Wigner function of the Hamiltonian of the ammonia system. after which, we will use the indicator of quantumness (or non-classicality) to control tunneling in this system. As we already know that Ammonia System is a tunneling system. In the work by Kenfack [6], he studied a simple indicator of non-classicality, which depend on the negative part of the Wigner function to explore few quantum state.

Similar quantities related to the volume of the negative part of theWigner function were used in [60, 62] to describe the interference effects which determine the departure from classical behaviour.

Furthermore, a closely related approach was recently advocated by Benedict and collaborators [63, 64]. Their measure of the non-classicality of a state $|\psi\rangle$ reads

$$v(\psi) = 1 - \frac{I_+(\psi) - I_-(\psi)}{I_+(\psi) + I_-(\psi)} \tag{2.3}$$

where $I_+(\psi)$ and $I_-(\psi)$ are the moduli of the integrals over those domains of the phase space where the Wigner function is positive and negative respectively. The normalization condition implies $I_+ - I_- = I_+$, so that $v = {}^{2I_-}/_{2I_- + 1}$ leads to $0 \leq v < 1$. Now, by using this notation, we may rewrite equation(2.2) as $\delta = I_+ + I_- - 1 = 2I_-$ and obtain a simple relation between both quantities.

$$v = \frac{2I_-}{1 + 2I_-} = \frac{\delta}{1 + \delta} \tag{2.4}$$

with $\delta = \frac{v}{1-v}$. It turns out that both quantities are equivalent in the sense that they induce the same order in the space of pure states: the relation $\delta(\psi_1) > \delta(\psi_2)$. However, from a practical point of view there exists an important difference between both quantities. To compute explicitly the quantity in equation (2.4), one faces a difficult task to identify appropriately the domains in which the integration has to be

carried out. In this indicator of quantumness proposed by Kenfack [6], by knowing the Wigner function $W(x, p)$ of a quantum state, one can easily and simply get its absolute value and evaluate numerically the integration in equation(2.2).

2.2.1 Test of Indicator of quantumness on Schr*ö*dinger cat state

The Schrödinger cat state owes its name to the Schrödinger's famous Gedankenexperiment [42]. In this experiment, the cat paradoxically turns out to be simultaneously in two macroscopically distinguishable states, namely dead and alive. The Schrödinger cat state is then defined as a superposition of two such states [37]. In Kenfack's work [6], he constructed similar 'cat states' by choosing two coherent states $\phi_{\pm}$ localized in two distant points of the configuration space, $\pm q_o$. The wavefunction of such a state reads in the position representation

$$\psi(q) = \frac{N}{\sqrt{2}} \left[\phi_+(q) + \phi_-(q)\right] \tag{2.5}$$

where

$$\phi_{\pm}(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}(q \pm q_o)^2 + i\frac{p_o}{\hbar}(q \pm q_o)\right) \tag{2.6}$$

the atomic units were used ($m = \hbar = \omega = 1$) in order words, the size of pq were measured in units of $\hbar$. The classical limit $\hbar \to 0$ means the action pq characteristic of the system many orders of magnitude larger than $\hbar$. equation (2.6) reveals that the phase, governed by p_o, is of great importance in that it induces oscillations on the wavefunction. It should be noted that the normalization constant N depends solely on the location of the centres (q_o, p_o) of both coherent states that make up the cat state. One can clearly see that the Wigner function may depend not only on the distance $2q_o$ between both states, but also on their momentum, p_o. So far, the studies on the cat states [34] have usually been restricted to the case of standing cats, p_o. In Kenfack's paper [6], he demonstrated that the parameter p_o influences the shape of the Wigner function, in particular, if $q_o \approx 1$ and both packets are not spatially related.

by inserting equation 2.6 into eqn 2.5, we obtain

$$W_{\psi}(q, p) = W_+(q, p) + W_-(q, p) + W_{int}(q, p) \tag{2.7}$$

here

$$W_{\pm}(q, p) = \frac{N^2}{2\pi} \exp(-(q \pm q_o)^2 - (p - p_o)^2) \tag{2.8}$$

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represents two peaks of the distribution centred at the classical phase point $(\pm q_o, p_o)$, while

$$W_{int}(q,p) = \frac{N^2}{\pi} \cos(2pq_o) \exp(-q^2 - (p - p_o)^2) \tag{2.9}$$

stands for the interference structure which appears between both peaks. Normalizing equation 2.2 yields

$$N = (1 + \cos(2p_o q_o) \exp(-q_o^2))^{-1/2} \tag{2.10}$$

making use of the equation 2.3 for the wigner function of the cat state $|\psi\rangle$, its non-classicality parameter is given as

$$\delta(\psi) = \iint | W_+(q,p) + W_{int}(q,p) + W_-(q,p) | \, dqdp - 1 \tag{2.11}$$

Check the appendix for detailed calculation of how this was solved and the python code I use to generate the result. In chapter 4, the results of the indicator of quantumness is displayed.

2.3   Double Well Potential

The double well potential has a number of applications; it is applied in the modelling of the ammonia potential [69] in studies involving ionization energy, quantum tunnelling to study a particle moving in a region of more than one constant potential [70] and ring puckering potential function, [71], where in chemistry a ring molecule is a molecule made up of several series of atoms bonded together to form a ring or cycle. Therefore ring puckering/gathering is the study that analyses the anharmonic energies that results from ring puckering/gathering vibrations. The double-well potential, though there are several functional forms, is usually in the form of,

$$V(x) = \alpha x^2 + \beta x^4$$

with $\alpha<0$, the barrier height and $\beta>0$,the steepness parameter. Despite the different functional forms of the double-well, the potential always has the following basic shape.
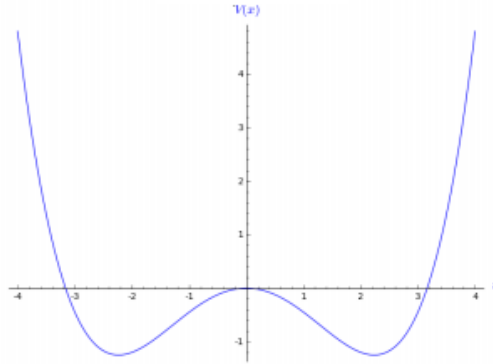
Figure 2.2: Double Well Potential

One notices that near the two local minima, the potential looks similarly to the harmonic potential. The height of the potential barrier at the center is represented by α but it is also affected by β, taken as the steepness parameter. As $\alpha \to \infty$the barrier height becomes infinite and the system decomposes into two independent components(almost harmonic potential but not, due to the quartic term), separated from each other. Harmoniously , the wave function of the system should tend to two split up sets of wave functions. If α is no longer infinite, a particle in either of the left or right hand region, has a non-zero tunnelling probability, that is tunnelling through the barrier to the other well. And therefore the wave functions for the left and right hand region are mixed with each other. Since the action will be symmetric ,$x \to -x$, the solutions for the Schrödinger equation can be broken up in to symmetric and antisymmetric wave functions. Usually the symmetric states have a lower energy compared to the antisymmetric states (since fewer number of nodes implies less kinetic energy for the particle). But this difference in lower energies is usually very small (slightly non-degenerate) and it gets more smaller and smaller as we increase α [72].

For instance, we take the example of Ammonia inversion. It is used to explain the inversion of the ammonia molecules, nitrogen and two hydrogen molecules. The hydrogen atoms forms a plane and at any given time, the nitrogen can be above or below the plane (quantum tunnelling). The position x, represent the position above or below this plane and the potential barrier is represented by the energy gap between the states of the positions of the nitrogen (above or below), see [73].

With the above arguments, we are bound to encounter interesting results, that there will be two slightly ordered pair non-degenerate energy levels for the system

This means that the wave functions for ordered pairs of eigenvalues will be symmetric and asymmetric of each other and this effect will be more pronounced at a larger barrier height. Using this well known argument, we use the matrix method to confirm them.

CHAPTER 3

METHODOLOGY

3.1 Ammonia System

The phenomenon of tunneling is investigated for symmetric double-well potential perturbed by a monochromatic driving force. The analysis is based on a numerical treatment of the quantum map that propagates the system over one period of the external force, and of the spectrum of its eigenphases (quasienergies). The variety in the quasienergy spectrum, such as exact and avoided crossings, leads to novel forms of tunneling. In 1927, Hund [] demonstrated that quantum tunneling is of importance for intramolecular rearrangements in pyramidal molecules such as ammonia, as manisfested by tunnel splitting of vibrational spectra. We want to study the influence of periodic on such tunnel model. The Hamiltonian defining the Ammonia System is

$$H(x,p) = \frac{p^2}{2} - \frac{1}{4}x^2 + \frac{x^4}{64D} \tag{3.1}$$

We make use of the dimensionless units. In the above expression, D is the barrier height and it is given as $D = \frac{E_B}{\hbar\omega_o}$. E_B is in units of $\hbar\omega_o$, with ω_o denoting the angular frequency of harmonic oscillations on the bottom of each well, and t is measured in units of the corresponding period $\frac{2\pi}{\omega o}$. This model Hamiltonian is of general interest: It characterizes the Physics of a wide class of systems, such as the transfer of hydrogen in atoms and molecules along chemical bond [65], the transport of hydrogen isotopes or muons between interstitial sites in metals [66] and macroscopic quantum coherence phenomena in SQUIDs [67, 68].

In this project, we attempt to gain insight into the deep quantum regime of this system. Meaning that we focus on the parameter range of low barriers, such that D is of order of unity and in the corresponding unperturbed problem, there are only a few levels below the barrier.The concept of autocorrelation function (i.e the probability to stay), local spectrum and quantum chaos was adopted.

3.2   Propagator of Hermitian operator

3.2.1   Time Dependence

The time evolution of any state is governed by Schrödinger's equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \tag{3.2}$$

It should be noted that in quantum mechanics, time, t, plays a fundamentally different role than the position, $\hat{q}$, or momentum, $\hat{p}$. The latter two are represented by operators that act on the states, while time is treated as a parameter. The state of the system depends solely on the parameter, t, but makes no sense to have a state that depends on an operator like $\hat{q}$. That is to say, $|\psi(t)\rangle$ is well defined but $|\psi(\hat{q})\rangle$ is not.

in most cases, the dependence on time t is understood and the short-hand version of the Schrödinger's equation:

$$i\hbar |\dot{\psi}_n\rangle = \hat{H} |\psi\rangle \tag{3.3}$$

Now, we want to know how the eigenstates of the Hamiltonian (i.e energy eigenstates) evolves with time. Applying Schrödinger's equation,

$$i\hbar |\dot{\psi}_n\rangle = \hat{H} |\psi_n\rangle = E_n |\psi_n\rangle \tag{3.4}$$

This is a first order differential equation for $|\psi_n(t)\rangle$ and it is easily verified that the general solution is:

$$|\psi_n(t)\rangle = e^{-\frac{iE_n t}{\hbar}} |\psi_n(0)\rangle \tag{3.5}$$

Thus, if the system starts in an energy state, it will remain in this eigenstate. The only effect of the time evolution is to multiply the state by a time-dependent phase factor $e^{-\frac{iE_n t}{\hbar}}$. Since an overall phase factor cannot influence the outcome of an observation, from an experimental perspective, energy eigenstates do no change with time. It is therefore a "stationary state". This motivates our interest in finding energy eigenstates for arbitrary Hamiltonians; any other state has the potential to change between observations, but a stationary state lives forever if we do not disturb it.

3.2.2   The Propagator Governs Time Evolution

It is trivial to determine $|\psi(t)\rangle$ if the system begins in a stationary state. The question is "What if the initial state is not an eigenfunction of the Hamiltonian?"

How do we evolve an arbitrary $|\psi(t)\rangle$ As we shown below, time evolution is governed by the propagator,

$$\hat{U}(t) \equiv e^{-\frac{i\hat{H}t}{\hbar}} \tag{3.6}$$

in terms of which the time evolved state is given by

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle \tag{3.7}$$

$\hat{U}(t)$ takes any state and evolves that state forward to time t according to the Schrödinger's equation.

3.3 Matrix Transformation for the Hamiltonian of Ammonia System

As already be defined, the hamiltonian of the Ammonia system reads

$$H(x,p) = \frac{p^2}{2} - \frac{1}{4}x^2 + \frac{x^4}{64D} \tag{3.8}$$

where D is the barrier height . It should also be noted that equation can be written as

$$H\psi_n = E\psi_n \tag{3.9}$$

Now, we need to solve equation (3.1) to get the eigenvalues and the corresponding eigenvectors. We start by setting

$$x = \frac{1}{\sqrt{2}}(a_+ + a_-) \quad and \quad p = \frac{d}{dx} = \frac{1}{\sqrt{2}}(a_- - a_+) \tag{3.10}$$

by substituting equation (3.4) into equation(3.1), we obtain

$$H(x,p) = -\frac{1}{4}(a_- - a_+)^2 - \frac{1}{4}\left(\frac{1}{\sqrt{2}}(a_+ + a_-)\right)^2 + \frac{1}{64D}\left(\frac{1}{\sqrt{2}}(a_+ + a_-)\right)^4 \tag{3.11}$$

$$H(x,p) = -\frac{1}{4}(a_- - a_+)^2 - \frac{1}{8}((a_+ + a_-))^2 + \frac{1}{256D}((a_+ + a_-))^4 \tag{3.12}$$

but

$$a_- = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix} \tag{3.13}$$

$$a_+ = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix} \tag{3.14}$$

$$a_- - a_+ = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & -\sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix} \tag{3.15}$$

in the same vein,

$$a_+ + a_- = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix} \tag{3.16}$$

Substituting equation(3.9) and (3.10) into equation 3.6, we obtain

$$H = -\frac{1}{4} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & -\sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix}^2 - \frac{1}{8} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix}^2$$

$$- \frac{1}{256D} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix}^4$$

as can be seen, the Hamiltonian of the Ammonia system has been transformed to the matrix form. To get the eigenvalues and the eigenvectors of this matrix analytically will be very difficult especially for highs dimension of the matrix. Analytically, I solved for $4X4, 3X3$, and $2X2$, matrices to get the eigenvalues and the corresponding eigenvectors. The results were confirmed analytically using Sagemath. After the confirmation of the results, we then extend to solve the eigenvalues and the corresponding eigenvectors of N dimension matrices. Where N can be any positive real number greater than one.

3.4 Sagemath code for the Numerical Solution of the Hamiltonian

Given that we are dealing with matrices, the first thing we have to do is to specify the dimensions of the matrix that we want to achieve. Let N represent the dimension. Note that we are only dealing with square matrices, N x N. But since we have matrices for the lowering, raising, and Hamiltonian matrix, it is best we start with defining the ladder operators first.

```
#modules that we will use for plotting the wave functions
import numpy as np
import math as m
###############################################################
def double_w2(N,n,D):
l_op=matrix(RDF,(N)) #creates an N by N matrix of zeros
#we then fill the initial matrix with the correct entries
for i in range(l_op.nrows()):
for j in range(l_op.ncols()):
if i <> j-1:
l_op[i, j] = 0
else:
l_op[i, j] = sqrt(j)
###############################################################
r_op=matrix(RDF,(N)) #creates an N by N matrix of zeros
#we then fill the initial matrix with the correct entries
for i in xrange(r_op.nrows()):
for j in xrange(r_op.ncols()):
```

```
if i <> j+1:
r_op[i, j] = 0
else:
r_op[i, j] = sqrt(j+1)
###########################################################
A=r_op+l_op;B=l_op-r_op
###########################################################
def H(A,B,list):
a=-0.25*B**(2) #evaluates the first part of the summation of H
b1=-0.125*A**(2)
b2=0.015625*0.2*D*A**(4)
return a+b1+b2
###########################################################
#calculates and returns the eigen values
def eva(A,B,list):
mat = H(A,B,list)
ls=mat.eigenvalues()
ls.sort()
return ls


###########################################################
#calculates and returns the eigen values
def evec(A,B,list):
mat = H(A,B,list)
ls=mat.eigenvectors_left()
ls.sort()
return ls


###########################################################
def coefficients(A,B,list,n):
eigenvectors = evec(A,B,list)
List = eigenvectors[n][1][0].list()
return List
###########################################################
###########################################################
```

```
def hermite(n):
var('x')
if n==0:
return 1
else:
return (-1)**(n)*np.exp(x**(2))*derivative(np.exp(-1*(x**(2))),x,n)
###########################################################
#wave functions for the simple Harmonic Oscillator
def wave_function(n):
pn = 1/(np.pi**(4))*(1/np.sqrt(2**(n)*m.factorial(n)))*hermite(n)*np.
    ↪ exp(-((x)**(2))/2)
return pn
###########################################################
def wave_function_new(A,B,list,n):
x = var('x') #variable x
CI = coefficients(A,B,list,n)
pn = 0 #iniatialises the wavefunctin, equation 1.3
for i in range(len(CI)):
pn = pn + CI[i]*wave_function(i)
return pn #the wavefunction for a given level n
############################################################
y = wave_function_new(A,B,[0,0,-1*D,0,0],n)
return plot(y,(x,-10,10),legend_label="Energy␣level␣%d" %(n), color =
    ↪ hue(0.1*n))
return evec(A,B,[0,0,-1*D,0,0.2])


def doub(N,n,D):
figure = graphics_array(((double_w2(N,n,D)+double_w2(N,n+1,D),
    ↪ double_w2(N,n+2,D)+double_w2(N,n+3,D)), (double_w2(N,n+4,D)+
    ↪ double_w2(N,n+5,D),double_w2(N,n+6,D)+double_w2(N,n+7,D)),(
    ↪ empty,empty)))
return figure.show(figsize = [10,10])


double_w2(30,0,4.3)
```

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Results of non-classicality indicator showing the quantumness of a Schrodinger Cat State

For Standing Cats $p_o = 0$
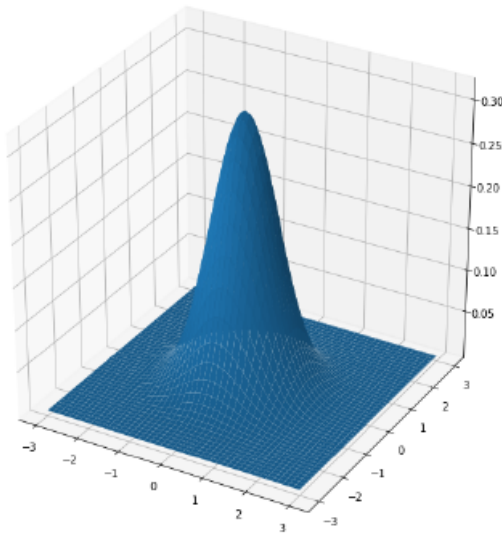
(a) $\delta = 0.0$, $(q_o, p_o) = (0, 0)$
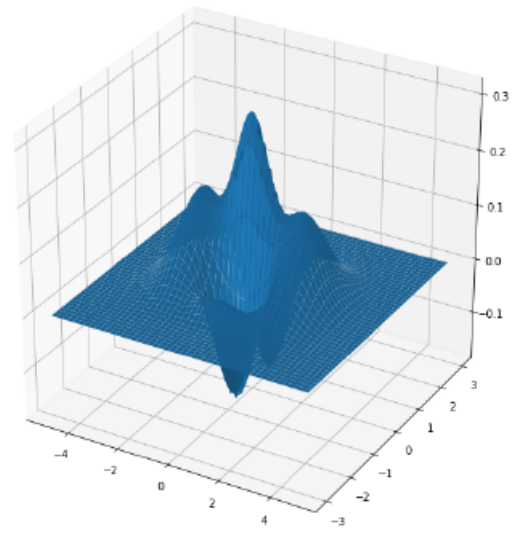
(b) $\delta = 0.421$, $(q_o, p_o) = (2, 0)$

For Standing Cats $p_o = 0$ / Cats in motion $p_o = 4$
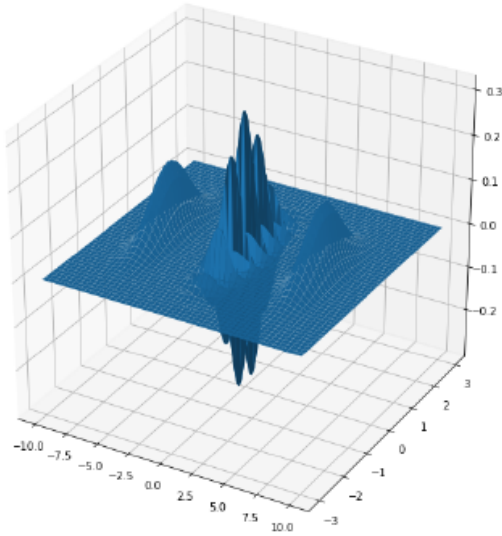
(a) $\delta = 0.636$, $(q_o, p_o) = (6, 0)$
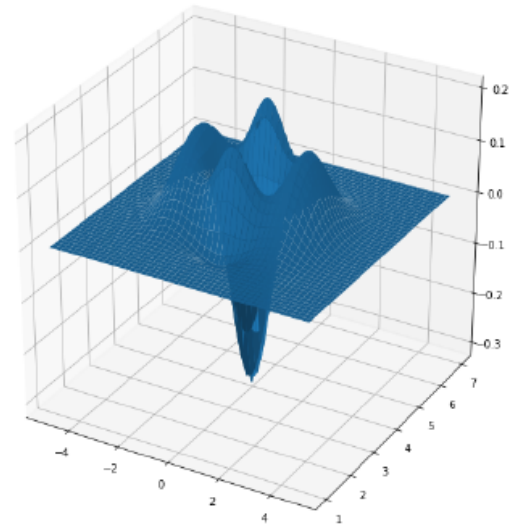
(b) $\delta = 0.491$, $(q_o, p_o) = (2, 4)$

For Standing Cats $p_o = 0$ / Cats in motion $p_o = 4$
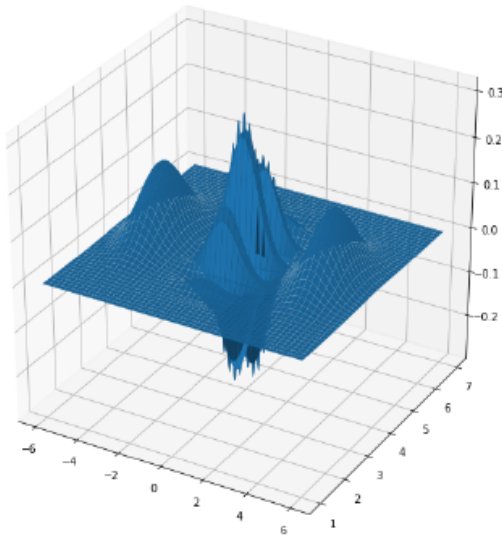
(a) $\delta = 0.630$, $(q_o, p_o) = (4, 4)$
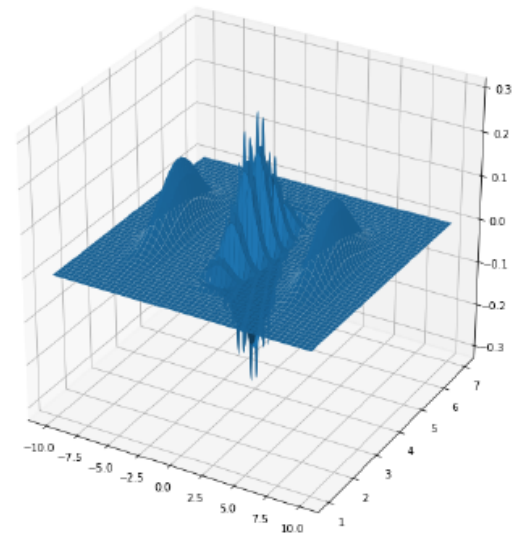
(b) $\delta = 0.636$, $(q_o, p_o) = (6, 4)$

Plot of Wigner function for which $\delta(q_o)$ achieves extremal values
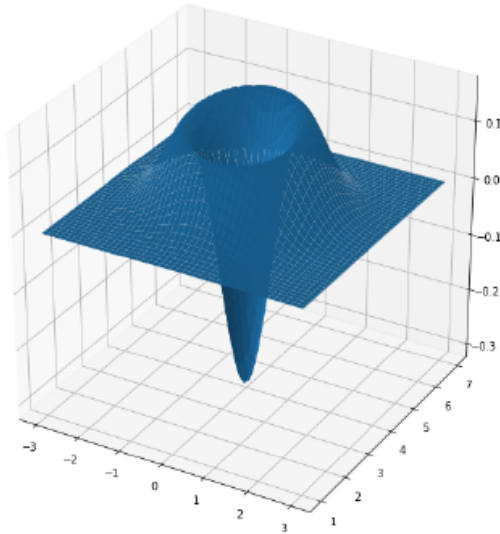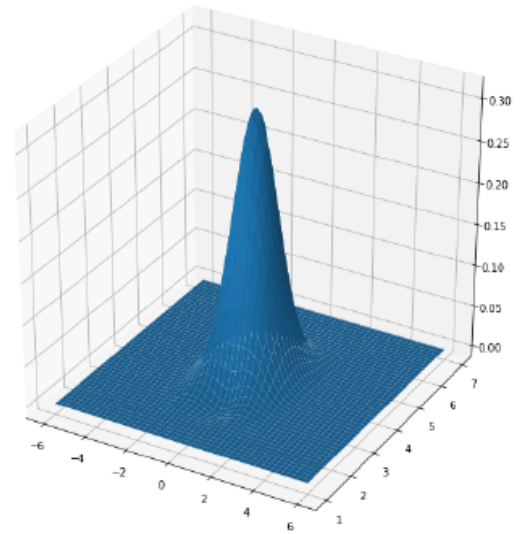
(a) $\delta = 0.420$, $\quad (q_o, p_o) = (0.4, 4)$

(b) $\delta = 0.01$, $\quad (q_o, p_o) = (0.725, 4)$

Plot of Wigner function for which $\delta(q_o)$ achieves extremal values
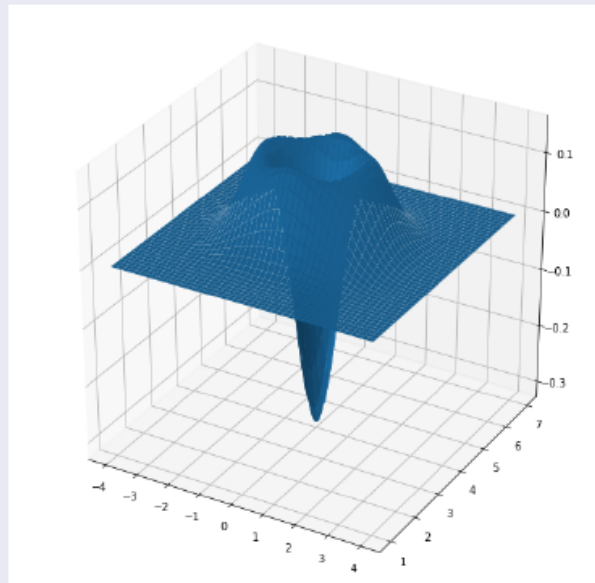
(a) $\delta = 0.420$, $\quad (q_o, p_o) = (1.175, 4)$

Plot of Wigner function for which $\delta(q_o)$ achieves extremal values
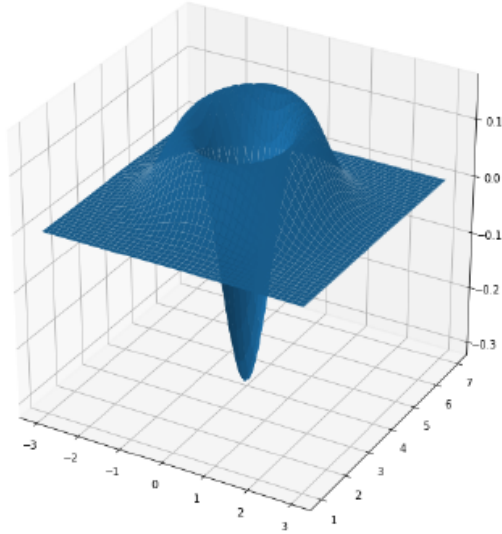
(a) $\delta = 0.420$, $(q_o, p_o) = (0.4, 4)$
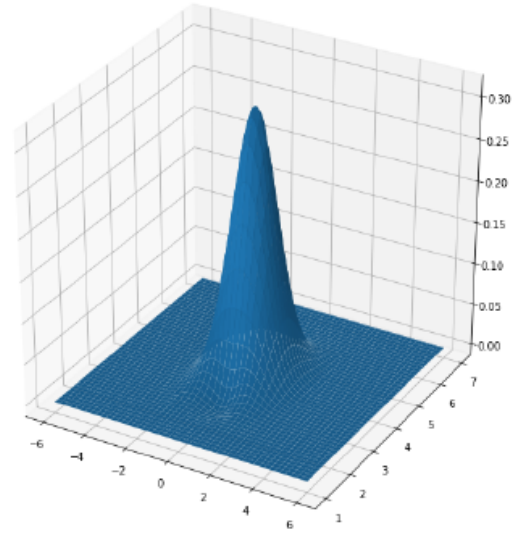
(b) $\delta = 0.01$, $(q_o, p_o) = (0.725, 4)$

The figures above showed the plots of the Wigner function of the cat states for several values of the separation q_o and the momentum p_o. One can clearly see the formation of the quantum interference structure halfway between the two humps as the separation distance q_o increases. The frequency of the interference structure increases with the separation. For intermediate separations $(0 < q_o \leqslant 4)$, the Wigner function changes its structure with p_o as shown in figure b and d above. In the case of standing cats $p_o = 0$, the indicator increases monotonically with the separation q_o, and reflects the presence of the interference pattern at $q_o = 0$. The growth of the nonclassicality saturates at $q_o \approx 4$, as the interference patterns become practically separated from both peaks, and parameter δ tends to the limiting value, $\delta_{max} \approx 0.636$.

The python code that generated this result is shown in Appendix A.2

4.2 EigenValues of the Ammonia System

level n	E_n, D = 0.6	E_n, D = 2	E_n, D = 4.3
0	-1.5996026637742005	-0.23989769946841885	0.0012448675099148107
1	-1.5994780323149402	-0.12851278556529844	0.34488305213777404
2	-0.7152002068804574	0.43741395914869696	1.065307812791431
3	-0.704970406885417	0.9631474872240787	1.8921767319973726
4	-0.06719356717834728	1.6242594500994405	2.8413659533604205
5	0.09635906023750233	2.3616186834033983	3.886202558206958
6	0.5309999381359086	3.1680579818635257	5.013748108452283
7	0.947046025019612	4.0345299851867615	6.214361610901761
8	1.4311467606023378	4.954813977345615	7.480794864195151
9	1.9529839490776302	5.924030685676718	8.80733437086849
10	2.5121734546719887	6.938268247431709	10.189397129349661
11	3.095945116482782	7.9942874397075325	11.62300451045438
12	3.3985971540757043	9.089398792751739	13.104879631918923
13	3.7257035502317892	10.220968279130082	14.610116948544468
14	4.380214090897581	11.387636815175291	16.163031369506054
15	5.05244572687154	12.175536535226875	16.205717169459685
16	5.754544754121348	12.636797546090813	17.82749951274338
17	6.4728743548878285	13.819056394996759	19.450967921247557
18	7.285860803321794	15.088447385269955	21.57570083504065
19	7.929372370597309	16.371194396304425	22.876645441747172
20	9.124294988624456	17.807873928097933	25.103192122682866
21	9.473971955551193	18.950681413254408	25.93480906613931
22	11.423929451766353	20.810227400611776	33.15582190346988
23	11.48021655325443824	22.11104785331129	34.138434499120734
24	14.170408285348529	23.729196139769414	47.33931810670286
25	14.326882571147868	23.94970916815751	48.31857639726889
26	17.72993260405349	30.0777454324631	70.06774712091088
27	18.076804496024288	30.730934415268457	71.03222640470486
28	22.73837588362689	45.42734282931892	108.9474217458324
29	23.306610978403505	46.271687862747854	109.90369723273429

Table 4.1: Table of eigenvalues,E_n, at different barrier heights D

From table (4.1), one can clearly see that as the Barrier is very small i.e D = 0.6, the system behaves exactly like double well potential having degeneracies. At D = 2, the system behaves exactly as Ammonia System having two bound state as can be seen from the result below. This result is generated by Fourier Grid Hamiltonian method. Check appendix A.3 and A.3.1 for more details.
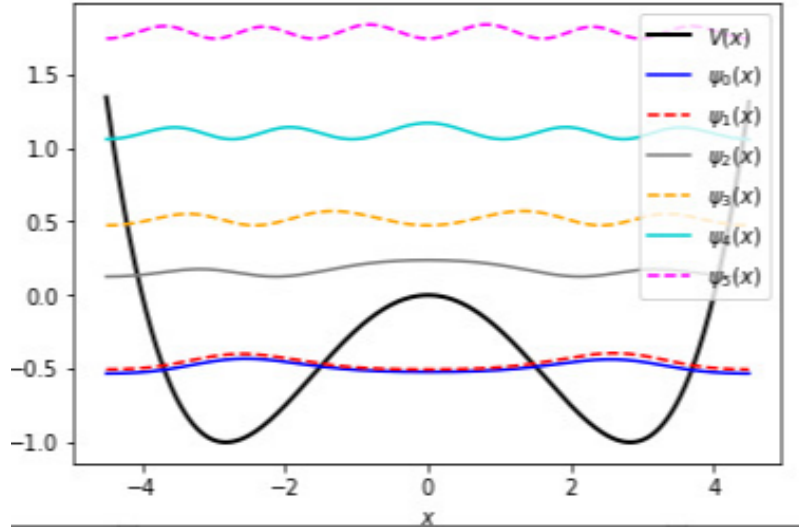
Finally as D becomes large, the system behaves exactly as Harmonic Oscillator (No bound states and No degeneracy). We now investigate the corresponding eigenfunctions/wave functions. The wave functions for ordered pairs of eigenvalues will be symmetric and asymmetric of each other and this effect will be more pronounced at a larger barrier height. Below are the results of wave functions for some energy levels.

When The ground state Energy is zero, we have the following results
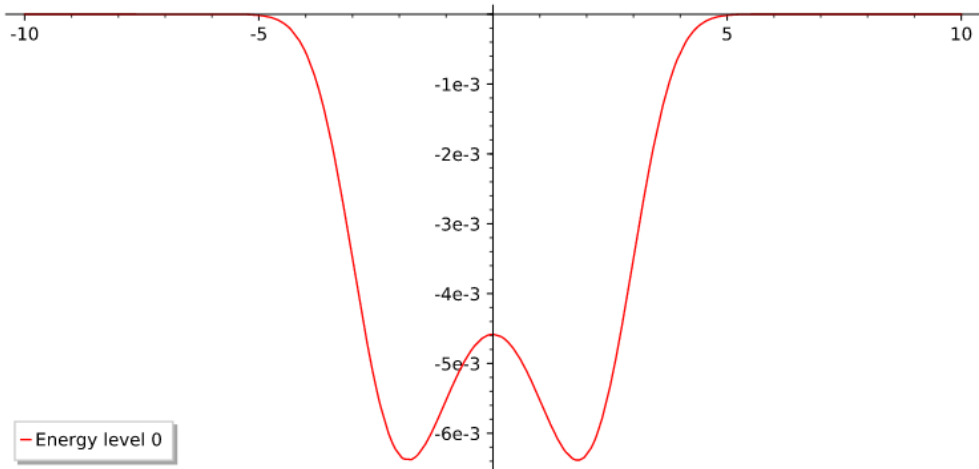
Figure 4.1: Wavefunction of Ammonia System for groundstate at D = 2
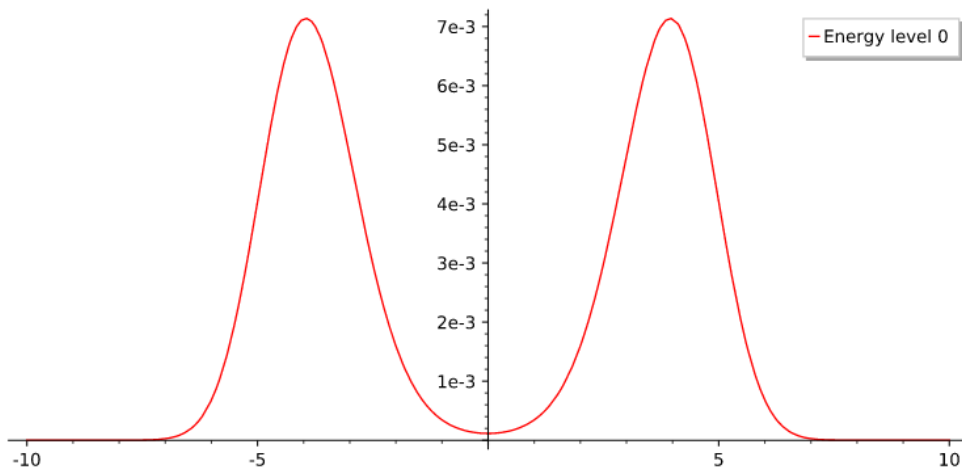
Figure 4.2: Wavefunction of Double Well System for groundstate at D = 0.6
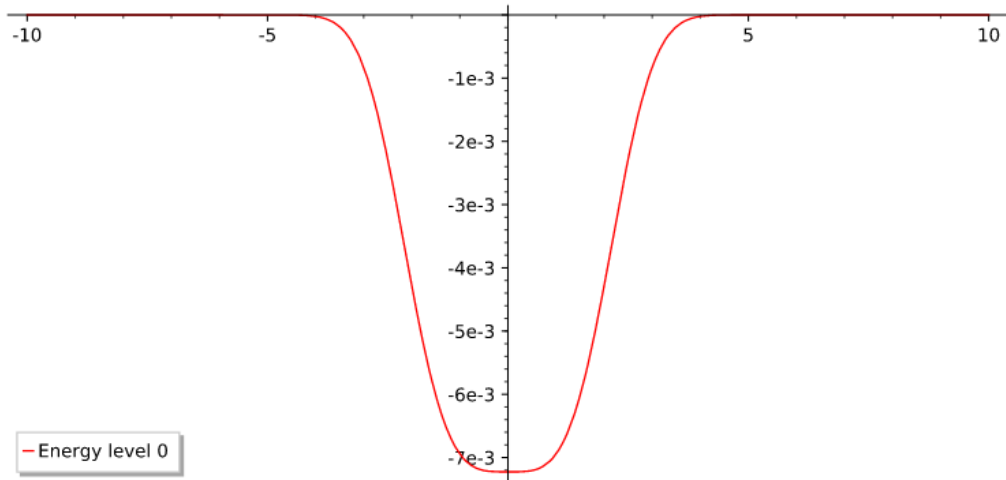
Figure 4.3: Wavefunction of Harmonic Oscillator for groundstate at D = 4.3

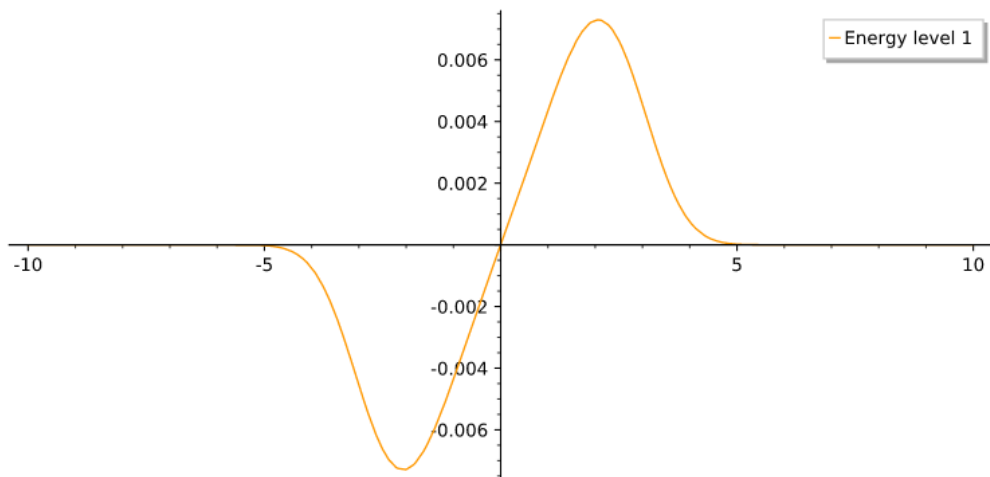For the first excited state energy, we have the following results

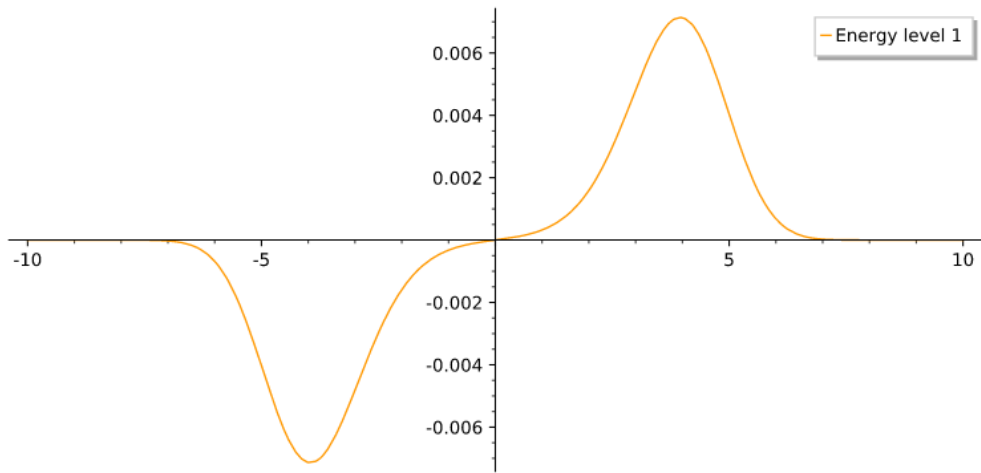**Figure 4.4:** Wavefunction of Ammonia for First excited state at D = 2

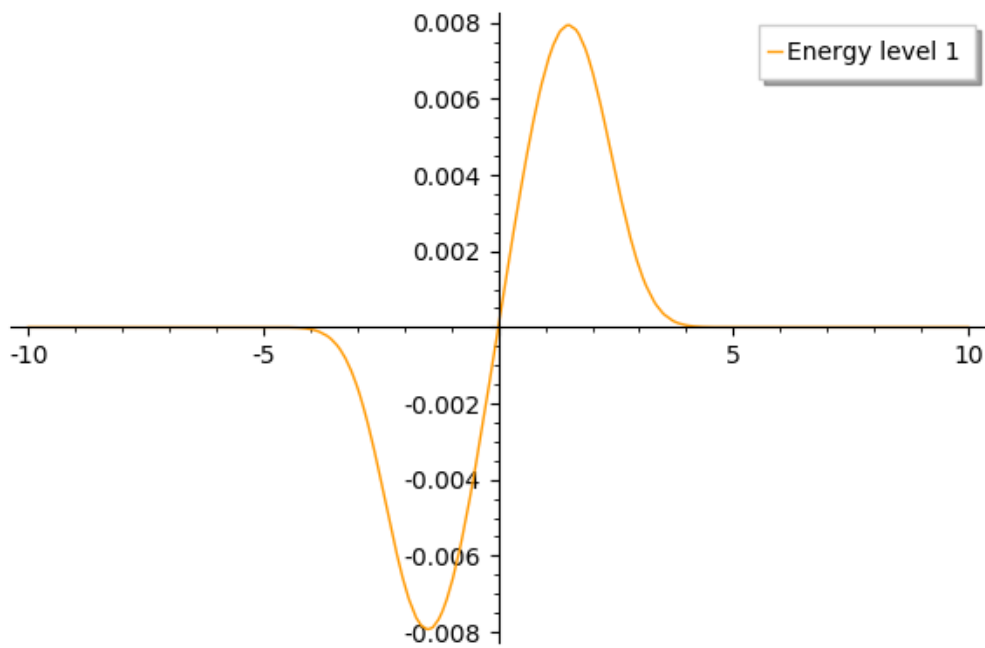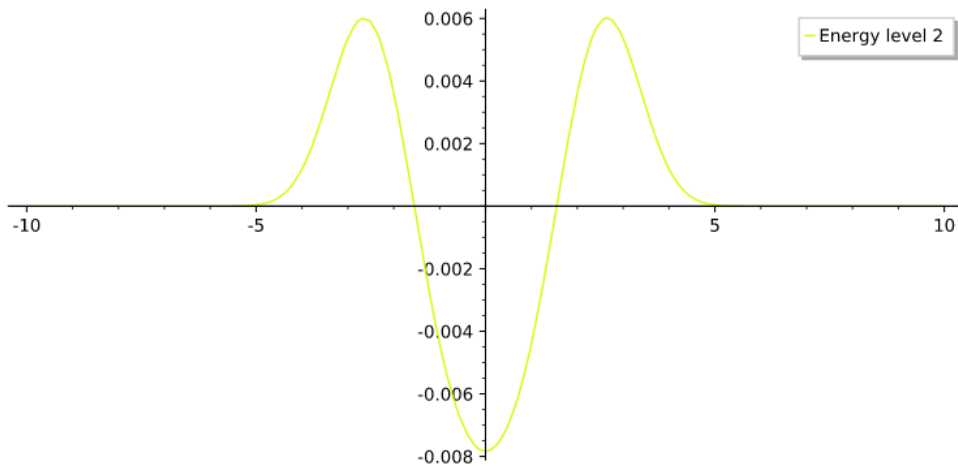**Figure 4.5:** Wavefunction of Double Well for First excited state at D = 0.6

Figure 4.6: Wavefunction of Harmonic Oscillator for First excited state at D = 4.3

For the second excited state energy, we have the following results

Figure 4.7: Wavefunction of Ammonia System for Second excited state at D =2
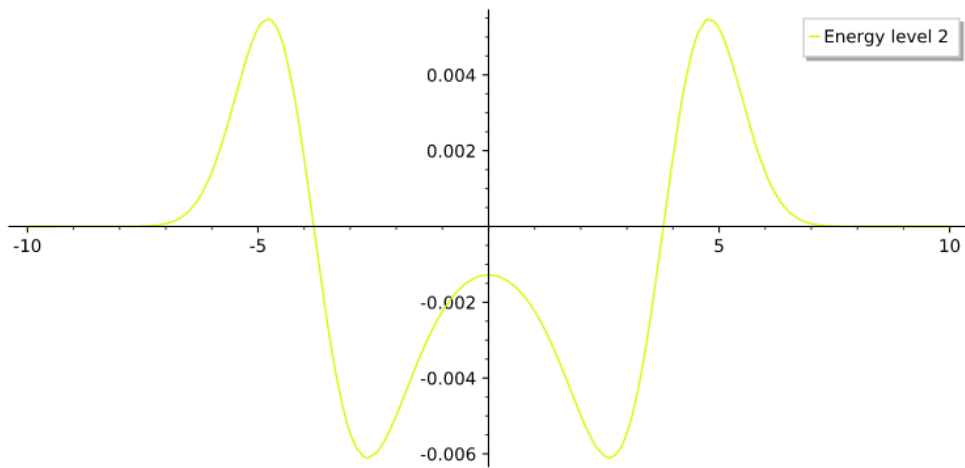

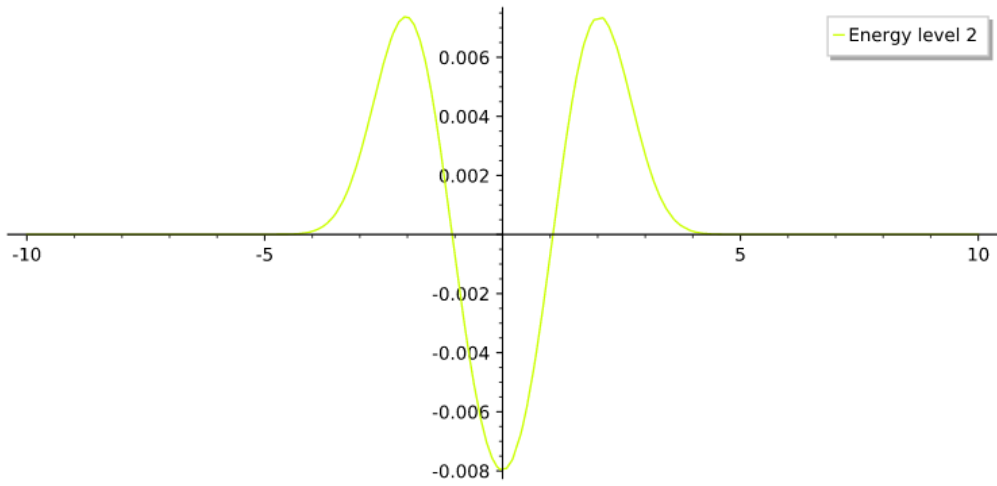**Figure 4.8:** Wavefunction of Double Well for Second excited state at D =0.6

Figure 4.9: Wavefunction of Harmonic Oscillator for Second excited state at D =4.3

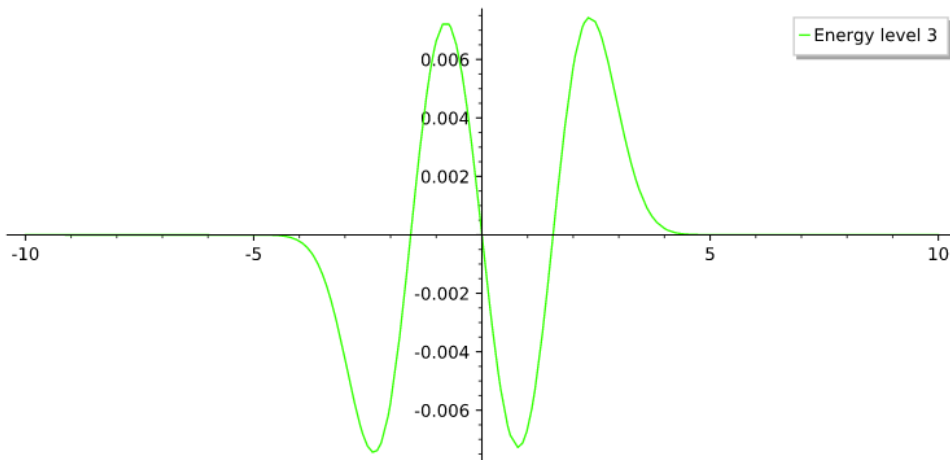For the Third excited state energy, we have the following results

Figure 4.10: Wavefunction of Ammonia System for Third excited state at D =2
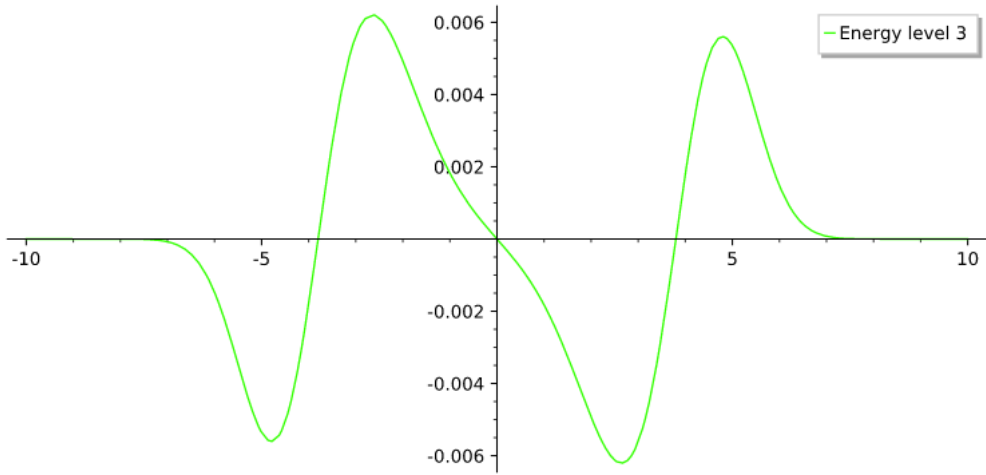
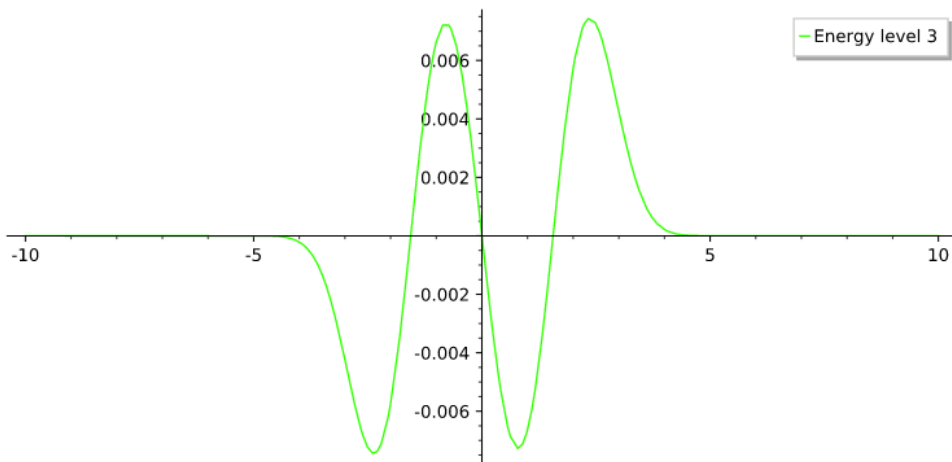**Figure 4.11:** Wavefunction of Double Well for Third excited state at D =0.6

Figure 4.12: Wavefunction of Harmonic Oscillator for Third excited state at D =4.3

The result of the quartic double well potential describing our system is shown
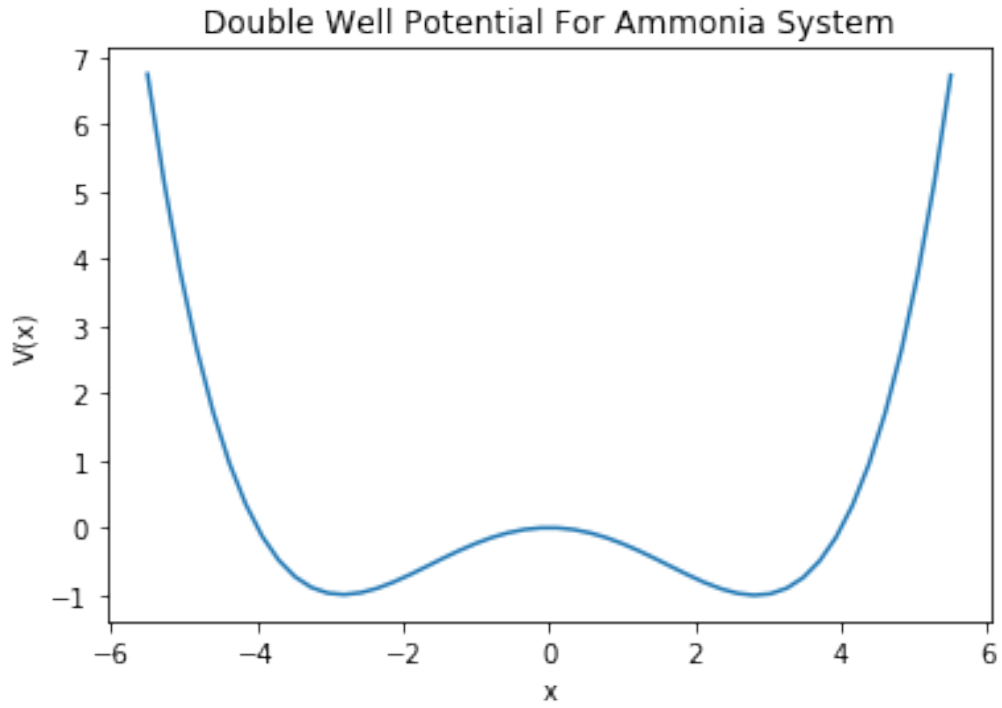
Figure 4.13: Double Well Potential

by setting an initial wavefunction at the left of the potential to be $\psi_{in} = \frac{1}{\sqrt{2}}(\psi_o - \psi_1)$ we obtained
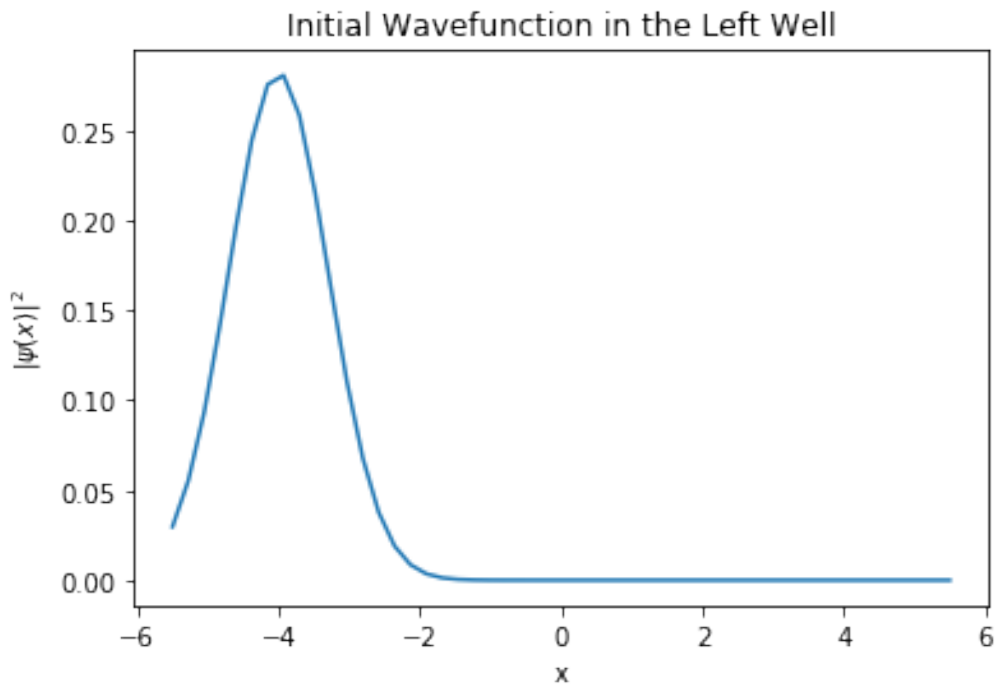

Figure 4.14: Double Well Potential

CHAPTER 5

CONCLUSION

What we are actually trying to do is to get the initial wavefunction and use a split operator method to get the evolution of the wavefunction. after which, we will get the corresponding Wigner Function of the evoluted wavefunction. We will then take the absolute squared of the Wigner Function since the indicator of non-classicality depends solely on this. Finally, this indicator of non-classicality will make us to have full control over tunneling in this system(i.e Ammonia System)

APPENDIX A

CODES AND CALCULATIONS

A.1 Detailed solution of Schrodinger cat state

$$\psi(q) = \frac{N}{\sqrt{2}} [\phi_+(q) + \phi_-(q)] \tag{A.1}$$

where

$$\phi_\pm(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} exp\left(-\frac{m\omega}{2\hbar}(q \pm q_o)^2 + \frac{ip_o}{\hbar}(q \pm q_o)\right) \tag{A.2}$$

using the atomic unit $m = \hbar = \omega = 1$, equation (2) can be written as

$$\phi_\pm(q) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} exp\left(-\frac{1}{2}(q \pm q_o)^2 + ip_o(q \pm q_o)\right) \tag{A.3}$$

but the Wigner Function of a state $|\psi\rangle$ is defined by

$$W_\psi(q,p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \left\langle q - \frac{x}{2} |\psi\rangle \langle\psi| q + \frac{x}{2} \right\rangle exp(ipx) \tag{A.4}$$

substituting equation (1) into equation (iv) gives

$$W_\psi(q,p) = \frac{N^2}{4\pi} \int_{-\infty}^{\infty} dx \left\langle q - \frac{x}{2} |\phi_+ + \phi_-\rangle \langle\phi_+ + \phi_-| q + \frac{x}{2} \right\rangle exp(ipx) \tag{A.5}$$

$$W_\psi(q,p) = \frac{N^2}{4\pi} \int_{-\infty}^{\infty} dx \left[\left\langle q - \frac{x}{2} |\phi_+\rangle \langle\phi_+| q + \frac{x}{2} \right\rangle + \left\langle q - \frac{x}{2} |\phi_+\rangle \langle\phi_-| q + \frac{x}{2} \right\rangle + \left\langle q - \frac{x}{2} |\phi_-\rangle \langle\phi_+| q - \right.\right.$$

$$\left. + \left[\left\langle q - \frac{x}{2} |\phi_-\rangle \langle\phi_-| q + \frac{x}{2} \right\rangle\right] exp(ipx) \right.$$

This can be written in a reduced form as

$$W_\psi(q,p) = \frac{N^2}{4\pi} \left\{ \int_{-\infty}^{\infty} dx I_1 + \int_{-\infty}^{\infty} dx I_2 + \int_{-\infty}^{\infty} dx I_3 + \int_{-\infty}^{\infty} dx I_4 \right\} exp(ipx) \tag{A.6}$$

$$W_1 = \int_{-\infty}^{\infty} dx I_1 exp(ipx), \quad W_2 = \int_{-\infty}^{\infty} dx I_2 exp(ipx), \quad W_3 = \int_{-\infty}^{\infty} dx I_3 exp(ipx), \quad and \quad so \quad on$$

where
$$I_1 = \left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle \left\langle \phi_+ \middle| q + \frac{x}{2} \right\rangle, \quad I_2 = \left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle \left\langle \phi_- \middle| q + \frac{x}{2} \right\rangle$$

$$I_3 = \left\langle q - \frac{x}{2} \middle| \phi_- \right\rangle \left\langle \phi_+ \middle| q + \frac{x}{2} \right\rangle, \quad I_4 = \left\langle q - \frac{x}{2} \middle| \phi_- \right\rangle \left\langle \phi_- \middle| q + \frac{x}{2} \right\rangle$$

Now, we want to solve I_1, I_2, I_3, I_4. Recall that from equation three we have

$$\phi_\pm(q) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} exp\left(-\frac{1}{2}(q \pm q_o)^2 + ip_o(q \pm q_o)\right)$$

Therefore

$$\left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} exp\left\{-\frac{1}{2}\left((q - \frac{x}{2}) + q_o\right)^2 + ip_o\left((q - \frac{x}{2}) + q_o\right)\right\}$$

$$\left\langle \phi_+ \middle| q + \frac{x}{2} \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} exp\left\{-\frac{1}{2}\left((q + \frac{x}{2}) + q_o\right)^2 - ip_o\left((q + \frac{x}{2}) + q_o\right)\right\}$$

$$\left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle \left\langle \phi_+ \middle| q + \frac{x}{2} \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} exp\left\{-\frac{1}{2}\left\{\left((q - \frac{x}{2}) + q_o\right)^2 + \left((q + \frac{x}{2}) + q_o\right)^2\right\} - ip_o x\right\}$$

$$I_1 = \left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle \left\langle \phi_+ \middle| q + \frac{x}{2} \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} exp\left\{-\left((q + q_o)^2 + \frac{x^2}{4}\right) - ip_o x\right\} \quad (A.7)$$

in the same vein,

$$I_2 = \left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle \left\langle \phi_- \middle| q + \frac{x}{2} \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} exp\left\{-\left(q^2 - \frac{x^2}{4}\right) + ip_o(-x + 2q_o)\right\} \quad (A.8)$$

also,

$$I_3 = \left\langle q - \frac{x}{2} \middle| \phi_+ \right\rangle \left\langle \phi_- \middle| q + \frac{x}{2} \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} exp\left\{-\left(q^2 - \frac{x^2}{4}\right) + ip_o(-x - 2q_o)\right\} \quad (A.9)$$

finally,

$$I_4 = \left\langle q - \frac{x}{2} \middle| \phi_- \right\rangle \left\langle \phi_- \middle| q + \frac{x}{2} \right\rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} exp\left\{-\left((q + q_o)^2 + \frac{x^2}{4}\right) - ip_o x\right\} \quad (A.10)$$

Therefore,

$$W_1 = \int_{-\infty}^{\infty} dx I_1 exp(ipx) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx exp\left\{-\left((q + q_o)^2 + \frac{x^2}{4}\right) - ip_o x\right\} exp(ipx)$$

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$$W_2 = \int_{-\infty}^{\infty} dx I_2 exp(ipx) = \frac{1}{\sqrt{\pi}} exp\left\{ -\left(q^2 - \frac{x^2}{4}\right) + ip_o(-x + 2q_o)\right\} exp(ipx)$$

$$W_3 = \int_{-\infty}^{\infty} dx I_3 exp(ipx) = \frac{1}{\sqrt{\pi}} exp\left\{ -\left(q^2 - \frac{x^2}{4}\right) + ip_o(-x - 2q_o)\right\} exp(ipx)$$

$$W_4 = \int_{-\infty}^{\infty} dx I_1 exp(ipx) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx exp\left\{ -\left((q - q_o)^2 + \frac{x^2}{4}\right) - ip_o x\right\} exp(ipx)$$

Recall

$$\int_{-\infty}^{\infty} exp(-\frac{1}{2}ax^2 + i\beta x)dx = \sqrt{\frac{2\pi}{a}} exp\left(-\frac{\beta^2}{2a}\right) \tag{A.11}$$

we then have

$$W_1 = 2e^{-(q+q_o)^2 - (p-p_o)^2} \tag{A.12}$$

$$W_2 = 2e^{2ip_o q_o} e^{-q^2 - (p-p_o)^2} \tag{A.13}$$

$$W_3 = 2e^{-2ip_o q_o} e^{-q^2 - (p-p_o)^2} \tag{A.14}$$

$$W_4 = 2e^{-(q-q_o)^2 - (p-p_o)^2} \tag{A.15}$$

Now, let's substitute W_1, W_2, W_3, W_4 into equation (6)

$$W_\psi(q,p) = \frac{N^2}{4\pi} \left[2e^{-(q+q_o)^2 - (p-p_o)^2} + 2e^{2ip_o q_o} e^{-q^2 - (p-p_o)^2} + 2e^{-2ip_o q_o} e^{-q^2 - (p-p_o)^2} + 2e^{-(q-q_o)^2 - (p-p_o)^2} \right] \tag{A.16}$$

$$W_\psi(q,p) = \frac{N^2}{2\pi} \left[e^{-(q+q_o)^2 - (p-p_o)^2} + e^{-(q-q_o)^2 - (p-p_o)^2} \right] + \frac{N^2}{\pi} \cos(2p_o q_o) e^{-q^2 - (p-p_o)^2} \tag{A.17}$$

A.2 Python code for Schrödinger cat state using indicator of non-classicality

```
import numpy as np
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
from matplotlib import cm
```

```python
dq = 0.01
dp = 0.01
q = [i for i in np.arange(-10,10+dq,dq)]
p = [j for j in np.arange(1,7+dp,dp)]

s1 = 0.0
q_0 = 6.0
p_0 = 4.0
N = (1+np.cos(2*p_0*q_0)*np.exp(-(q_0)**2))**-0.5
for i in range(len(q)):
for j in range(len(p)):
s1+= abs(N**2/(2*np.pi)*(np.exp(-(q[i]+q_0)**2 - \
(p[j]-p_0)**2))+N**2/(2*np.pi)*(np.exp(-(q[i]-q_0)**2 - (p[j]-p_0)
    ↪ **2))+\
N**2/np.pi*np.cos(2*p[j]*q_0)*np.exp(-q[i]**2-(p[j]-p_0)**2))

s1 = s1*dq*dp
print(s1-1.0)



fig = plt.figure(figsize=(10,10))
ax = fig.add_subplot(111, projection='3d')

# Make data.
N = (1+np.cos(2*p_0*q_0)*np.exp(-(q_0)**2))**-0.5
q, p = np.meshgrid(q, p)

W1 = N**2/2*np.pi*(np.exp(-(q+q_0)**2 - (p-p_0)**2))
W2 = N**2/2*np.pi*(np.exp(-(q-q_0)**2 - (p-p_0)**2))
W3 = N**2/2*np.pi*(2*np.cos(2*p*q_0)*np.exp(-(q)**2-(p-p_0)**2))
W = W1 + W2 + W3
print(type(W))
```

```
# Plot the surface.
surf = ax.plot_surface(q, p, W)


# Customize the z axis.
ax.set_xlabel('q')
ax.set_ylabel('p')
ax.set_zlabel('W')


plt.show()
```

A.3 The Fourier Grid Hamiltonian method

The method computes the matrix elements of the kinetic energy operator in position
representation analytically. For position-dependent potentials, the potential energy
operator is diagonal in position representation. Both terms are added to obtain the
symmetric Hamiltonian matrix, which is diagonalised to obtain both eigenvalues and
eigenvectors (wavefunctions in position representation).

A.3.1 Fourier Grid Hamiltonian Code

```
from itertools import cycle


import numpy as np
import matplotlib.pyplot as plt
from scipy.linalg import eigh
from scipy.integrate import simps


%load_ext Cython


%%cython


# cython: boundscheck=False
# cython: cdivision=True
# cython: wraparound=False
```

```python
import numpy as np
cimport numpy as np


cpdef H_cont(double L, double[:] V):


cdef int N = len(V)
cdef np.ndarray[dtype=double, ndim=2] Hij = np.zeros([N, N])
cdef double K, pi = np.pi
cdef int i, j


K = pi/(L/N) # pi/dx


for i in range(N):
for j in range(i+1):
if i == j:
Hij[i, j] = 0.5*K**2/3. + V[i]
else:
Hij[i, j] = K**2/pi**2 * (-1.)**(j-i)/(j-i)**2
Hij[j, i] = Hij[i, j] # use Hermitian symmetry


return Hij


pot = lambda x: x**4/64 - x**2/4 # potential function callable


N = 2**10 # number of samples in discretization
L = 10. # length of x support
x_vals = np.linspace(-L/2, +L/2, N, endpoint=False)


V_sampled = pot(x_vals)
H_sampled = H_cont(L, V_sampled)


# diagonalize the Hamiltonian matrix:
E, psi = eigh(H_sampled)


# quick and dirty visualization:
```

```python
N_plot_min = 0 # quantum number of first eigenfunction to plot
N_plot = 6 # number of eigenfunctions to plot


WF_scale_factor = (np.max(V_sampled) - np.min(V_sampled))/N_plot
plt.plot(x_vals, V_sampled, ls="-", c="k", lw=2, label="$V(x)$")


style_cycler = cycle(["-", "--"]) # line styles for plotting
color_cyler = cycle(["blue", "red", "gray", "orange", "darkturquoise"
    ↪ , "magenta"])


for i in range(N_plot_min, N_plot_min+N_plot):
# physically normalize WF (norm = 1)
WF_norm = simps(np.abs(psi[:,i])**2, x=x_vals)
psi[:,i] /= np.sqrt(WF_norm)
# higher energy --> higher offset in plotting
WF_plot = WF_scale_factor*np.abs(psi[:,i])**2 + E[i] # also try
    ↪ plotting real part of WF!
plt.plot(x_vals, WF_plot, ls=style_cycler.next(), lw=1.5, color=
    ↪ color_cyler.next(),
label="$\psi_{}(x)$".format(i))
print("E[%s]␣=␣%s"%(i, E[i]))


plt.xlabel("$x$")
plt.legend(loc="best")
plt.show()
```

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