Wigner and Husimi Distribution Functions for Quantum Systems

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Certificate of Examination

This is to certify that the dissertation titled **Wigner and Husimi Distribution Function for Quantum Systems** submitted by **Mr. Sandeep Singh (Reg. No. MS13079)** for the partial fulfillment of BS-MS dual degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Dr. Sanjeev Kumar   Dr. Rajeev Kapri   Dr. P. Balanarayan (Supervisor)

Dated: April 26, 2019

Declaration

The work presented in this dissertation has been carried out by me with Dr. P. Balanarayan at the Indian Institute of Science Education and Research Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

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In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. P. Balanarayan
(Supervisor)

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Sandeep Singh

“All our knowledge begins with the senses, proceeds then to the understanding, and ends with reason. There is nothing higher than reason.”

Immanuel Kant

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Abbreviations

a.u.	**a**tomic **u**nits
WF	**W**igner **F**unction
HF	**H**usimi **F**unction
HO	**H**armonic **O**scillator
QDF	**Q**uantum **D**istribution **F**unction
DVR	**D**iscrete **V**ariable **R**epresentation

Dedicated to my Family.

Abstract

The present work deals with the study of Wigner and Husimi function for quantum systems. We have applied Wigner function to the Harmonic oscillator and represented it in the phase space distribution. We have proposed two different methods to compute the Wigner function using fourier transformation. We are applying these methods to model quantum systems and later calculating the electron densities for atoms and molecules.

Chapter 1

Wigner Distribution Function

1.1 Introduction

Wigner function (WF) was first introduced by Eugene P. Wigner in 1932. "Wigner used these functions to find the quantum corrections to classical statistical mechanics where the Boltzmann factor contains energy, which in turn are expressed as functions of both position and momentum" [1]. Later it was used to study the relation between the quantum mechanical quantities and their corresponding classical quantities. It is also used in understanding semi-classical quantum mechanics [2].

Wigner distribution function is a quantum distribution function (QDF). It includes functions that depend on both coordinate and momenta. It is real and can be normalized to one. It can be positive as well as negative whereas a regular distibution function is always positive. A necessary condition on wigner function, for it to be strictly non negative is when the wavefunction of the considered system is a minimum uncertainity wave function [3]. Negative region of the wigner distribution can be smoothed out by averaging over a coarse graining function to obtain a Husimi distribution function (HF), which is also a QDF [4].

WF and HF both are quasiprobability distribution. WF gives correct probability densities but it is a quasiprobability distribution because it gives negative values at some regions of the phase space whereas HF has non-negative distribution but its not a true probability distribution because it does not produce correct probability densities [5].

According to classical hamiltonian physics, a state for variables in position and momentum space is given by a point in a 6N dimensional phase space. The Uncertainty principle is not valid in classical physics, thus it is possible to know a particle's momentum and position simultaneously to an arbitrary precision, which is not possible in quantum mechanics. Probability densities of the wavefunction in position basis and in momentum basis are used in the standard formulation of quantum mechanics.

Non-relativistic quantum mechanics in phase space can be mathematically described using wigner function. WF can be considered equivalent to the standard quantum mechanics, if we only look at wavefunction and schrodinger equation in the case of non-relativistic quantum mechanics. But, WF formulates quantum mechanics in phase space same as hamiltonian mechanics, therefore is much more closely related to the classical mechanics [3].

Due to the unique nature of WF, classical approach and entanglement in quantum approach and observing deviation from classical behaviour becomes easy and intesering. Information obtained from experimentally reconstructed WF exceeds the information on the system by any other method. It is used in various field such as quantum processing (as it is perfect to illustrate the quantum properties of entanglement), quantum physics (to model the electron transport), quantum electronics and also in quantum chemistry where it is used to calculate static and dynamic properties of many body quantum system [6].

1.2 Formulation

Time dependent WF associated with a pure state $\Psi(x,t)$ is:

$$W(x,p,t) = \frac{1}{2\pi\hbar}\int \exp\left(\frac{ipq}{\hbar}\right)\Psi^*\left(x+\frac{q}{2},t\right)\Psi\left(x-\frac{q}{2},t\right)dq. \tag{1.1}$$

Time independent WF associated with a pure state $\Psi(x)$ [2] is:

$$W(x,p) = \int \left(\frac{dq}{2\pi}\right) \exp\left(\frac{ipq}{\hbar}\right) \Psi^*\left(x + \frac{q}{2}\right) \Psi\left(x - \frac{q}{2}\right), \tag{1.2}$$

where integration limits are $-\infty$, ∞.

WF has a proper marginal distribution i.e. the integral over one set of variables of the wigner function gives the square modulus of the function in the representation assoaciated with the remaining variable. marginal distribution for WF is given as:

$$\int dpW(x,p) = |\Psi(x)|^2 \tag{1.3}$$

$$\int dxW(x,p) = |\Phi(p)|^2. \tag{1.4}$$

Here, $\Phi(p)$ is the wavefunction in the momentum representation and $\Psi(x)$ is the wavefunction in the position representation.

The HF is given by,

$$H(x,p) = \frac{1}{b\sqrt{2\pi}} \times \left| \int \frac{dq}{\sqrt{2\pi\hbar}} \Psi(q) \exp\left(\frac{-1}{4b^2}(x-q)^2 + \frac{ipq}{\hbar}\right) \right|^2 \tag{1.5}$$

where parameter b is arbitrary and associated with the width of the gaussian. HF is positive everywhere, but does not follow proper marginal distribution.

$$\int dpW(x,p) \neq |\Psi(x)|^2 \tag{1.6}$$

$$\int dxW(x,p) \neq |\Phi(p)|^2 \tag{1.7}$$

1.3 Properties of Wigner Function

Mathematical properties of WF [3]:

1. If the wavefunction $\psi(x,t)$ is normalized to one then WF for the wavefunction given by $W(x,p,t)$ is also normalized to one.

$$\int\int \psi(x,t)dpdx = 1 \implies \int\int W(x,p,t)dpdx = 1 \tag{1.8}$$

furthermore, the equation

$$\int W(x,p,t)^2 dpdx = \frac{1}{2\pi\hbar} \tag{1.9}$$

holds for all pure states $\psi(x,t)$.

2. Quantum Mechanical probability densities in position and momentum space may be obtained from the marginals of the WF:

$$\rho(x,t) = \int dpW(x,p) = |\Psi(x)|^2 \tag{1.10}$$

$$\rho(p,t) = \int dxW(x,p) = |\Phi(p)|^2 \tag{1.11}$$

3. The state overlap of two wave function $\psi_1(x,t)$ and $\psi_2(x,t)$ in terms of their WF $w_1(x,p,t)$ and $w_2(x,p,t)$ is :

$$\int \psi_1^*(x,t)\psi_2^*(x,t)dx = 2\pi\hbar \int w_1(x,p,t)w_2(x,p,t)dpdx \tag{1.12}$$

4. The WF obeys the reflection symmetries:

$$\psi(x,t) \rightarrow \psi^*(x,t) \implies w(x,p,t) \rightarrow w(x,-p,t) \tag{1.13}$$

$$\psi(x,t) \rightarrow \psi(-x,t) \implies w(x,p,t) \rightarrow w(-x,-p,t) \tag{1.14}$$

5. The WF is Galilei-covariant , i.e.

$$\psi(x,p,t) \rightarrow \psi(x+y,p,t) \implies w(x,p,t) \rightarrow w(x+y,p,t) \tag{1.15}$$

1.4 Plan of thesis

WF is capable of visualizing quantum mechanics in phase space representation for a given system. Wigner and HF for the quartic oscillator in a double well potential was done by Marcel Novaes [2]. We have tested the WF for Harmonic oscillator (HO) to produce a phase space representation and studied its properties. WF basically does the fourier transform of a function with a shift in the position coordinate. Our goal is to find the phase space properties of atoms and molecules. Fourier transformation of a function takes the function from position basis to momentum basis, vice-versa and enables us to obtain electron density and electron momentum density of an atom or a molecule.

For appplying WF on HO, we derive the HO wave function with the shift of $\pm q/2$ and compute hermite polynomial with this shift. Where q is the shift in position coordinate 'x' of HO. To solve WF for HO we have used subroutine for the 'Gauss Legendre' method of integration. For the electron density [7], We propose the hypothesis that 'fourier transform with the Wigner shift can be estimated by taking a matrix multiplication of a function with the kinetic energy eigenfunction matrix'.

In chapter 2, We discuss and understand the mathematical methods and calculations used to compute the WF for the HO. In chapter 3, plots and discussion for the phase space representation of WF for the HO and conclusion of above mentioned hypothesis are mentioned.

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Chapter 2

Mathematical Methods

2.1 Double Well Potential

Double-well potentials have been extensively studied and used in the different fields of physics and chemistry for the description of the motion of a particle under two centers of force [1]. In classical mechanics, a particle with energy less than the central potential barrier in any of the well (minima) can never leave the well whereas quantum mechanics allows the particle to tunnel through the barrier and appear in the other well, this phenomenon is known as the tunneling effect. WF and HF, associated with the stationay states of double well potential show that the low energy states are highly non-classical, due to the tunneling effect [2].

The associated stationary Schrӧdinger equation for double well quantum systems:

$$\left(\frac{-1}{2}\left(\frac{d^2}{dx^2}\right) - \frac{\beta}{2}x^2 + x^4\right)\Psi_n(x) = e_n\Psi_n(x) \tag{2.1}$$

is dimensionless and β controls the height of the barrier [5]. The classical analogue of equation (2.1) is solvable analytically and given as:

$$\left(\frac{1}{2}\left(\frac{dx}{dt}\right)^2 - \frac{\beta}{2}x^2 + x^4\right) = E. \tag{2.2}$$

We have used discrete variable representation (DVR) method (Appendix A) to solve for the double well potential. The double well potential and the eigen vectors are produced and plotted figure 2.1 and figure 2.2.

In figure 2.1 the first four enegy levels of a quantum Harmonic oscillator are plotted along with the potential for $\beta = 0$. In this case double well behaves as a single well and therefore we observe an increase in the oscillations with each increasing value of quantum number 'n'.

In figure 2.2 we have plotted the first four energy levels of the double well potential for $\beta = 10$. In this case, we observe the tunneling and tunnel splitting of the particle in a double well potential. The degenracy between the first and second energy levels, third and fourth energy levels are seen for $\beta = 10$.

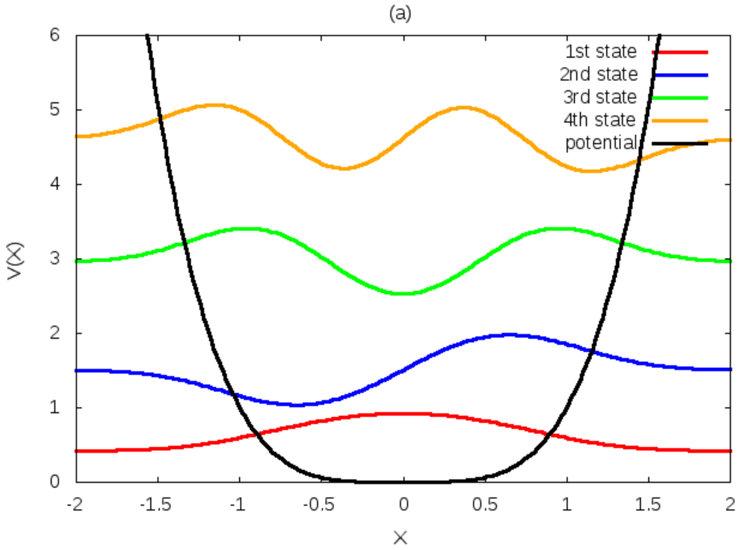

Figure 2.1: First four enegy levels of Harmonic Oscillator visualised for a double well potential for β=0.

2.2 Particle in a Box

The particle in a infinite box, is a quantum mechanical model, which consists of a particle moving horizontally within an infinitely deep well (infinte potential at the boundaries) from which it cannot escape. The potential energy in this model is given

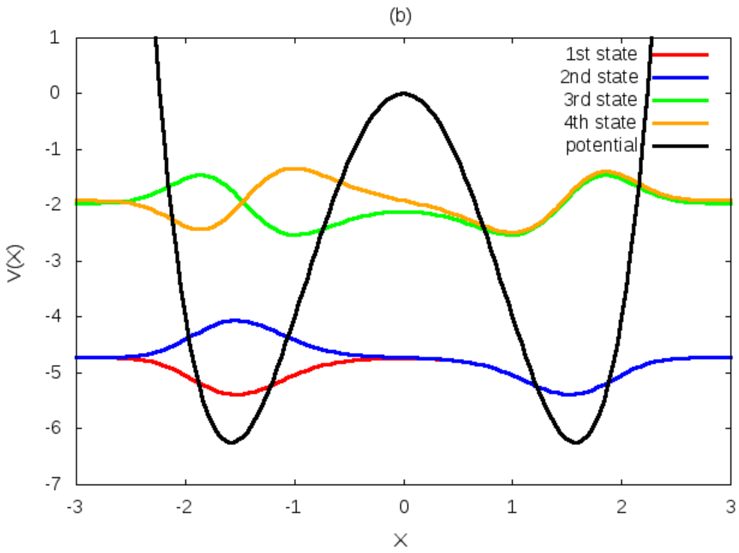

FIGURE 2.2: First four enegry levels of Harmonic Oscillator visualised for a double well potential for β=10.

as:

$$V(x) = \begin{cases} 0, & x_c - \frac{L}{2} < x < x_c + \frac{L}{2} \\ \infty, & \text{otherwise} \end{cases} \tag{2.3}$$

where L is the length of the box, x_c lies at the center of the box and x is the position of the particle in the box.

Particle in a box wave functions are given by:

$$\psi_n(x,t) = \sqrt{\frac{2}{L}}\sin(kx)e^{-iE_nt/\hbar} \tag{2.4}$$

$$\tag{2.5}$$

where $k = n\pi/L$, E_n is the energy of the nth state and t is the time.

In figure 2.3 and 2.4, the real and imaginary part of the particle in box wave function of length $L = 20$ $a.u.$ for the ground state are plotted, along with the complete wave function in the position and momentum basis, respectively.

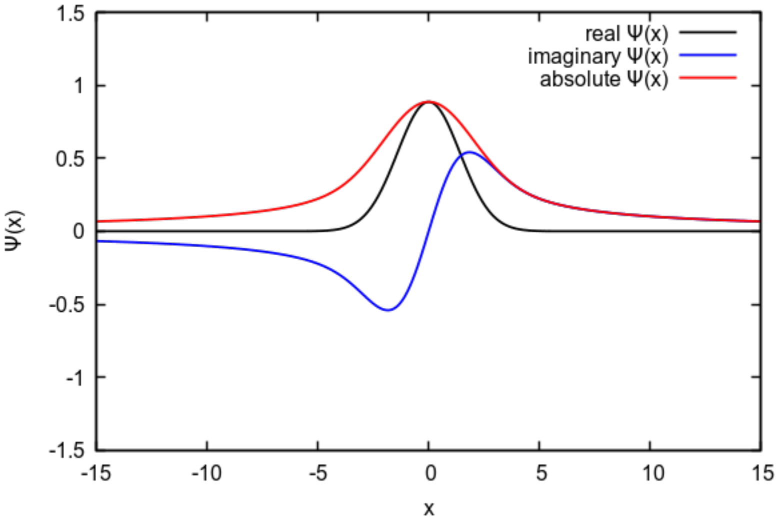

FIGURE 2.3: Particle in a box wave function in positon basis.

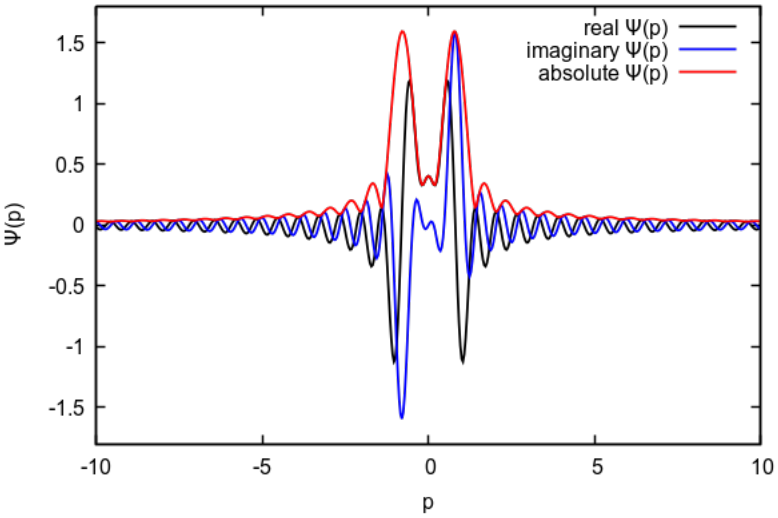

FIGURE 2.4: Particle in a box wave function in momentum basis.

2.3 Harmonic Oscillator

In classical physics a Harmonic oscillator is described as a physical system in which when a particle is displaced from the equilibrium it experiences a restoring force which is proportional to the displacement. At sufficiently small energies, the laws of quantum mechanics govern the Harmonic oscillator, where the system is known as quantum oscillator [3]. The energy of the classical Harmonic oscillator can take any non-negative value whereas the quantum Harmonic oscillator has only discrete energy levels which are given by:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{2.6}$$

where $\hbar$ is the Planck's constant, ω is a classical angular frequency and n is a positive integer that determines the state. The Hamiltonian for the Harmonic oscillator is given by:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mw^2}{2}\hat{x}^2. \tag{2.7}$$

where m is mass of the particle, $\hat{p}$ is momentum operator and $\hat{x}$ is position operator. The Schrödinger equation for the stationary state of the Harmonic oscillator is:

$$\left(\frac{\hat{p}^2}{2m}\right)\Psi + \frac{1}{2}mw^2\hat{x}^2\Psi = E\Psi. \tag{2.8}$$

and its solution is the wave function:

$$\Psi_n(x) = A\frac{1}{\sqrt{2^n n!}}H_n(x)\exp(\frac{-x^2}{2}) \tag{2.9}$$

where n is the state, A is a normalization constant given by:

$$A = \left(\frac{mw}{\pi\hbar}\right)^{1/4} \tag{2.10}$$

and $H_n(x)$ is a Hermite Polynomial [4].

The Fourier transform of (2.8) takes the domain from position representation to the momentum representation, which is given by:

$$\psi_n(p) = \left(\frac{1}{\pi\hbar mw}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\frac{p}{\sqrt{\hbar mw}}\right)\exp\left(-\frac{p^2}{2\hbar mw}\right). \tag{2.11}$$

2.3.1 Hermite Polynomials

Hermite polynomials (HPs) are a set of orthogonal polynomials over the domain (-∞,∞) with a weighting function. Solutions of the Hermite's differential equation are also known as the HPs [3], which are defined as:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n e^{-x^2}}{dx^n}. \tag{2.12}$$

The first few HPs are representated as:
$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_3(x) = 8x^3 - 12x$
$H_4(x) = 16x^4 - 49x^2 + 12.$
In figure 2.5 we have shown the first five Hermite polynomials against the position coordinate.

Recurrence Relation: A Hermite polynomials at one point can be obtained by neighboring HP at the same point. HPs recurrence relation is given as:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{2.13}$$

and its differential form is:

$$\frac{\partial H_n(x)}{\partial x} = 2nH_{n-1}(x). \tag{2.14}$$

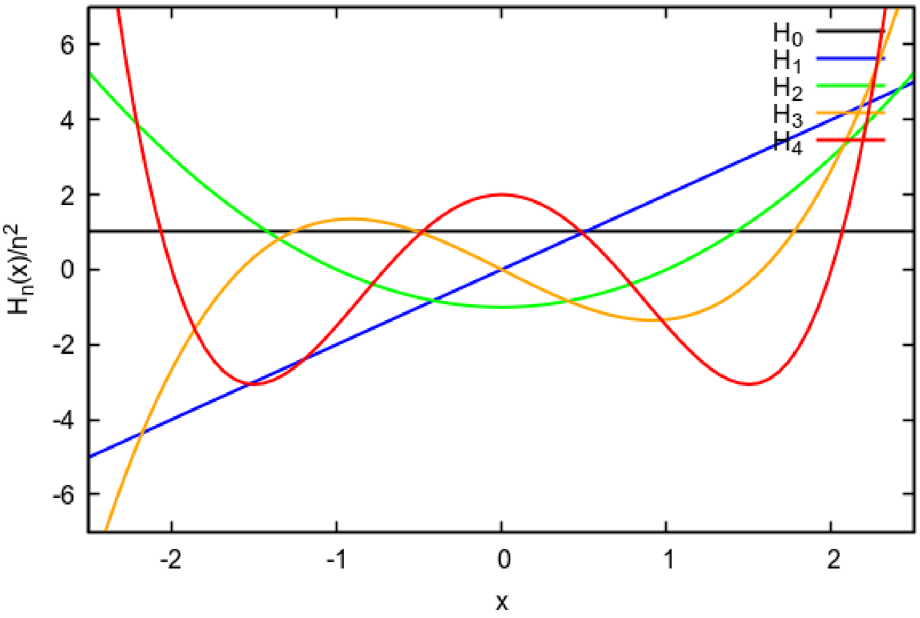

FIGURE 2.5: First five Hermite polynomial scaled down by a factor of n^2 in order to fit on the same plot.

2.4 Wigner Function for the Harmonic Oscillator

In this section, we have done the calculation to compute Wigner Function for the Harmonic oscillator. The Wigner Function is represented as:

$$W(x,p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp\left(\frac{ipq}{\hbar}\right)\Psi^*\left(x+\frac{q}{2}\right)\Psi\left(x-\frac{q}{2}\right)dq, \tag{2.15}$$

where Ψ is a wave function of a pure state and Ψ^* is a complex conjugate wave function of Ψ.

As the wave functions for the Harmonic oscillator are real, the complex conjugate $\psi^*(x)$ is equal to $\psi(x)$. The form of the wave function is:

$$\Psi_n(x) = \Psi_n^*(x) = A\frac{1}{\sqrt{2^n n!}}H_n(x)\exp(\frac{-x^2}{2}). \tag{2.16}$$

According to the definition of the WF, to compute the WF for the HO the x coordinate of the HO wave functions $[\psi_n(x)]_{n=0}^{\infty}$, is shifted by $\pm q/2$. The modified HO wave functions are given as:

$$\Psi_n^*\left(x+\frac{q}{2}\right) = A\frac{1}{\sqrt{2^n n!}}H_n\left(x+\frac{q}{2}\right)\exp\left(\frac{-(x+\frac{q}{2})^2}{2}\right) \tag{2.17}$$

$$\Psi_n\left(x-\frac{q}{2}\right) = A\frac{1}{\sqrt{2^n n!}}H_n\left(x-\frac{q}{2}\right)\exp\left(\frac{-(x-\frac{q}{2})^2}{2}\right). \tag{2.18}$$

The product of the equation (2.17) and equation (2.18) is:

$$\Psi^*(x+\frac{q}{2})\Psi(x-\frac{q}{2}) = A^2\frac{1}{2^n n!}H_n\left(x+\frac{q}{2}\right)H_n\left(x-\frac{q}{2}\right)\exp\left(-\frac{(x+q/2)^2}{2}\right) \exp\left(-\frac{(x-q/2)^2}{2}\right). \tag{2.19}$$

The first part of the equation (2.19) $A\frac{1}{\sqrt{2^n n!}}$ is the normalization constant, where $A = (mw/\pi\hbar)^{1/4}$. The second part of the equation $(H_n(x+q/2)\ H_n(x-q/2))$ are the shifted Hermite polynomials and the third part is exponential part of the HO wave function with a shift of $\pm q/2$. To compute the first part we need to calculate A^2. In atomic units ($m = w = \hbar = 1$), A becomes $(1/\pi)^{1/4}$ and therefore $A^2 = (1/\pi)^{1/2}$. Puting the value of A^2 back in equation (2.19), we get:

$$\Psi^*(x+\frac{q}{2})\Psi(x-\frac{q}{2}) = \frac{1}{\sqrt{\pi}}\frac{1}{2^n n!}H_n\left(x+\frac{q}{2}\right)H_n\left(x-\frac{q}{2}\right)\exp\left(-\frac{(x+q/2)^2}{2}\right) \exp\left(-\frac{(x-q/2)^2}{2}\right). \tag{2.20}$$

The exponential part is solved, using the fundamental multiplicative identity for exponentials ($e^a e^b = e^{a+b}$). We obtain the following equation:

$$\Psi^*(x+\frac{q}{2})\Psi(x-\frac{q}{2}) = \frac{1}{\sqrt{\pi}}\frac{1}{2^n n!}H_n\left(x+\frac{q}{2}\right)H_n\left(x-\frac{q}{2}\right)\exp\left(-\frac{(x+q/2)^2}{2}-\frac{(x-q/2)^2}{2}\right). \tag{2.21}$$

After simplifying:

$$\Psi^*(x+\frac{q}{2})\Psi(x-\frac{q}{2}) = \frac{1}{\sqrt{\pi}}\frac{1}{2^n n!}H_n\left(x+\frac{q}{2}\right)H_n\left(x-\frac{q}{2}\right)\exp\left(-x^2-\frac{q^2}{4}\right). \tag{2.22}$$

To solve the second part of the equation we need to compute $H_n(x+q/2)$ and $H_n(x-q/2)$, which are the shifted Hermite Polynomials. The Hermite Polynomials reccurence relation now takes the form:

$$H_{n+1}\big(x+\frac{q}{2}\big) = 2\big(x+\frac{q}{2}\big)H_n\big(x+\frac{q}{2}\big) - 2nH_{n-1}\big(x+\frac{q}{2}\big) \tag{2.23}$$

$$H_{n+1}\big(x-\frac{q}{2}\big) = 2\big(x-\frac{q}{2}\big)H_n\big(x-\frac{q}{2}\big) - 2nH_{n-1}\big(x-\frac{q}{2}\big). \tag{2.24}$$

We have assigned the following values to the initial hermite polynomials with the shift of $\pm q/2$,
$H_0\big(x+\frac{q}{2}\big) = 1$
$H_0\big(x-\frac{q}{2}\big) = 1$
$H_1\big(x+\frac{q}{2}\big) = 2\big(x+\frac{q}{2}\big)$
$H_1\big(x-\frac{q}{2}\big) = 2\big(x-\frac{q}{2}\big)$
and used the reccurence relation given in (2.23) and (2.24) to the find the rest of Hermite Polynomials. After putting equation (2.22) in equation (2.15) we get:

$$W(x,p) = \frac{1}{\pi^{1/2}}\frac{1}{2^n n!}\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ipq}\exp\big(-x^2-\frac{q^2}{4}\big)H_n\big(x+\frac{q}{2}\big)H_n\big(x-\frac{q}{2}\big)dq. \tag{2.25}$$

Now we have an integral equation over -∞ to ∞. To solve this integral we have written a code in fortran based on 'Gauss Legendre' method for integration. We have also used a simple integration technique to solve equation (2.25). After successfully computing the WF for HO, we plot it for two cases (p=0 and $p \neq 0$) which we will discuss in chapter 3.

2.5 Electron Density

The electron density (ED), is the probability of an electron being present at a specific location. In quantum calculations ED $\rho(\vec{r})$ is a function that depends on the coordinates $\vec{r}$. It is defined so $\rho(\vec{r})dr$ is the number of electrons present in th volume

dr. The charge density $\rho(\vec{r})$ is defined in terms of the many-particle wave function, $\Psi(\vec{r_1}, \vec{r_2}, \vec{r_3}, .., \vec{r_N})$ as:

$$\rho(\vec{r}) = N \int \left|\Psi(\vec{r_1}, \vec{r_2}, \vec{r_3}, .., \vec{r_N})\right|^2 d^3r_2 d^3r_3 ....d^3r_N. \tag{2.26}$$

The electron momentum density (EMD), $\gamma(\vec{p})$ is a single particle charge denstiy in the momentum space. The momentum space wave function, $\Phi(\vec{p_1}, \vec{p_2}, \vec{p_3}, .., \vec{p_N})$ is obtained by a Fourier transform of the position space wave function, $\Psi(\vec{r_1}, \vec{r_2}, \vec{r_3}, .., \vec{r_N})$. EMD is given as:

$$\gamma(\vec{p}) = N \int \left|\Phi(\vec{p_1}, \vec{p_2}, \vec{p_3}, .., \vec{p_N})\right|^2 d^3p_2 d^3p_3 ....d^3p_N. \tag{2.27}$$

The densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ are positive semi-definite and normalize to the number of electrons present in the system [5]:

$$\int \rho(\vec{r}) d^3r = \int \gamma(\vec{p}) d^3p = N. \tag{2.28}$$

2.5.1 Fourier Transform

Fourirer Transform (FT) is defined as a mathematical tool, which is used to construct a given function into the sum of simple sinusoidal functions.

The quantum phenomenon can be considered in the position domain '$f(x)$' or the momentum domain '$F(p)$' and it is possible to go from $f(x)$ to $F(p)$ by the means of a Fourier transform which is given by the relation [6]:

$$F(p) = \int_{-\infty}^{\infty} f(x) e^{-ipx} dx. \tag{2.29}$$

Whereas, inverse Fourier transform takes the domain from F(p) to f(x), which is given as:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(p) e^{ipx} dp. \tag{2.30}$$

2.5.2 Fourier Transform of the Gaussian basis

A general gaussian type orbital is given by:

$$\chi(\vec{r}) = N_r(x-x_a)^{l_x}(y-y_a)^{l_y}(z-z_a)^{l_z} \tag{2.31}$$

$$\exp\Big[-\alpha\big((x-x_a)^2+(y-y_a)^2+(z-z_a)^2\big)\Big] \tag{2.32}$$

$$N_r = (2\pi\alpha)^{3/4}\left(\frac{(4\alpha)^{\frac{l_x+l_y+l_z}{2}}}{(2l_x-1)!!(2l_y-1)!!(2l_z-1)!!}\right)^{1/2} \tag{2.33}$$

Discrete Fourier transform (DFT) on the Guassian basis results in the Fourier transformed momentum space representation, which is given by:

$$\chi(\vec{p}) = N_p\sum_{k_1=0}^{l_x/2}\frac{(-1)^{k_1}(p_x/\sqrt{\alpha})^{l_x-2k_1}}{k_1!(l_x-2k_1)!}\sum_{k_2=0}^{l_y/2}\frac{(-1)^{k_2}(p_y/\sqrt{\alpha})^{l_y-2k_2}}{k_2!(l_y-2k_2)!} \tag{2.34}$$

$$\sum_{k_1=0}^{l_z/2}\frac{(-1)^{k_3}(p_z/\sqrt{\alpha})^{l_z-2k_3}}{k_3!(l_z-2k_3)!} \tag{2.35}$$

$$N_p = \frac{i^{l_x+l_y+l_z}}{(2\pi\alpha)^{3/4}}\left(\frac{(4\alpha)^{\frac{l_x+l_y+l_z}{2}}}{(2l_x-1)!!(2l_y-1)!!(2l_z-1)!!}\right)^{-1/2} \tag{2.36}$$

$$l_x!l_y!l_z!\exp(\frac{-\vec{p}^2}{4\alpha}+i\vec{p}.\vec{A}) \tag{2.37}$$

where α is exponent for a gaussian.l_x, l_y, l_z are the components of angular momentum and x_a, y_a, z_a are position of atoms in three dimensional space [5].

2.5.3 WF calculations using Fourier Transform

Wigner function provides us the Fourier transform of a wave function with the shift of $\pm q/2$. To compute this transform we have to do an integratration on q for each and every value of x, which is rather complicated. Irrespective of what wave function we use, we have to accompy the shift on 'x' co-ordinate for integration on 'q' over $(-\infty,\infty)$.

The WF associated with a state $\psi(x)$ resembles a Fourier transform of the state $\psi(x)$ and is given as:

$$W(x,p) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp\left(\frac{ipq}{\hbar}\right)\Psi^*\left(x+\frac{q}{2}\right)\Psi\left(x-\frac{q}{2}\right)dq. \tag{2.38}$$

DFT of a wave function $\psi_n(x \pm q/2)$ is given as:

$$F(p) = \int_{-\infty}^{+\infty} e^{-ipq}F(q) \tag{2.39}$$

where $F(q) = \psi_n^*(x+q/2)\psi_n(x-q/2)$. It can also be writen as:

$$F(p) = \sum_{n=0}^{\infty} F(q) \tag{2.40}$$

From above, we can find the values of momentum coordinate (p) for fixed a value of position coordinate (x). This transformation should be equivalent to the transformation produced by the WF.

We propose two different ways in which we can compute the Fourier transform with the shift given for the WF of $\pm q/2$. One way to achieve the transformation is by multiplying the wave function with the eigen vectors of the kinetic energy matrix generated using DVR (Appendix A) method [7]. Second method is to multiply the wave function with the Fourier grid hamiltonian matrix which is given as:

$$M = \begin{bmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & W & W^2 & W^3 & \dots & W^{N-1} \\ 1 & W^2 & W^4 & W^6 & \dots & W^{N-2} \\ 1 & W^3 & W^6 & W^9 & \dots & W^{N-3} \\ \vdots & & & & & \\ 1 & W^{N-1} & W^{N-2} & W^{N-3} & \dots & W \end{bmatrix}$$

where $W = \exp(-i2\pi/N)$.

To acheive the Fourier transform with the shift similar to that of WF, we followed the following procedure :

1. First step is to write the HO wave function with the shift of $\pm/2q$.
2. In first method, we multiply the eigen vectors of the kinetic energy matrix to a HO wave wave function and then we compare the result with WF for the HO.
3. In second method, Fourier grid hamiltonian matrix is multiplied with the HO wave function and then we compare the result with WF for the HO.
4. A code is written in fortran to accomplish the matrix multiplication and test the hypothesis mentioned above.

Results and conclusions are discussed in the chapter 3.

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Chapter 3

Results and Discussions

In the previous chapter we have shown how to compute the WF for the HO and described two methods by which we can compute WF using Fourier transform. In this chapter we will discuss the results and conclusions for the work done so far.

3.1 Visualizing Wigner Distribution Function for the Harmonic oscillator

The final form of the WF for the HO is given as:

$$W(x,p) = \frac{1}{\pi^{1/2}} \frac{1}{2^n n!} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ipq} \exp\big(-x^2 - \frac{q^2}{4}\big) H_n\big(x + \frac{q}{2}\big) H_n\big(x - \frac{q}{2}\big) dq. \quad (3.1)$$

It can also be written in the submission form as:

$$W(x,p) = \frac{1}{\pi^{1/2}} \frac{1}{2^n n!} \frac{1}{2\pi} \sum_{j=1}^{n} e^{ipq} \exp\big(-x_j^2 - \frac{q^2}{4}\big) H_n\big(x_j + \frac{q}{2}\big) H_n\big(x_j - \frac{q}{2}\big) \omega_j \quad (3.2)$$

where x_i and ω_i are gaussion quadrature roots and weights, respectively. To plot the WF for the HO, we wrote a code in fortran using two differnt methods. In one we used a 'Gauss Legendre' method to solve for the integral and in other we used a 'simple integration technique'. Both methods produce the same output, which we used to plot the phase space distribution of WF for the HO.

3.1.1 WF for HO in position Basis

Wigner distribution function for the HO is plotted against the position coordinate keeping the momentum coordinate $p = 0$, corresponding to the stationary state of harmonic oscillator. In figure 3.1, we see a cut through the plane $p = 0$ of the ground

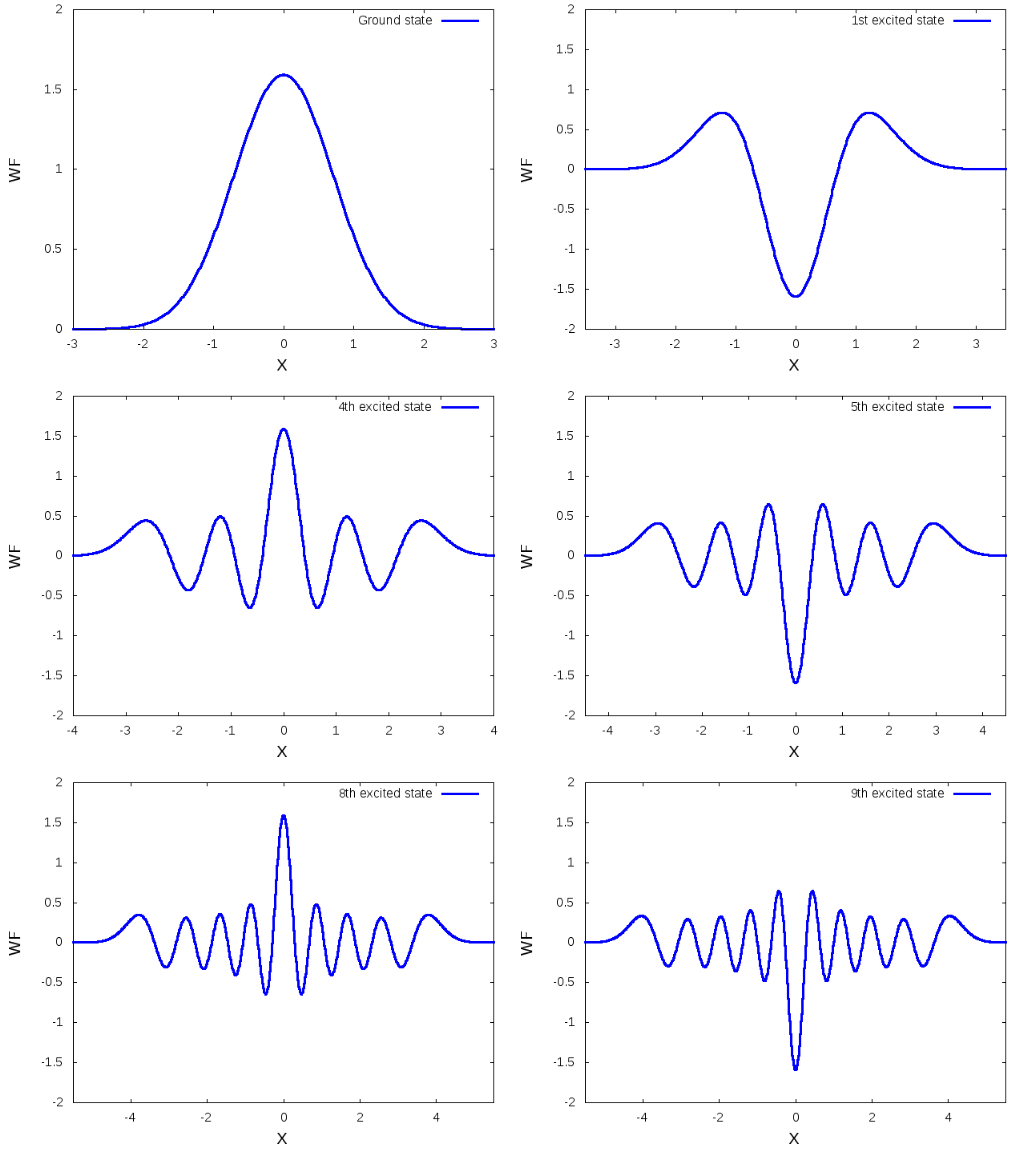

FIGURE 3.1: WF for the HO is plotted agaist the position coordinate for ground state and first excited state, fourth and fifth excited state, eighth and ninth excited state for $p = 0$.

state and first excited state WF for the HO. Next plots represents fourth, fifth, eighth and ninth excited state WF for the HO. In ground state the function is positive everywhere. Whereas, through first and ninth excited state we find the distribution to be psoitive as well as negative.

3.1.2 Phase Space Representation of WF for HO

Phase space representation of WF for the HO (real $W(x, p)$) are shown for the case where, momentum $p \neq 0$.

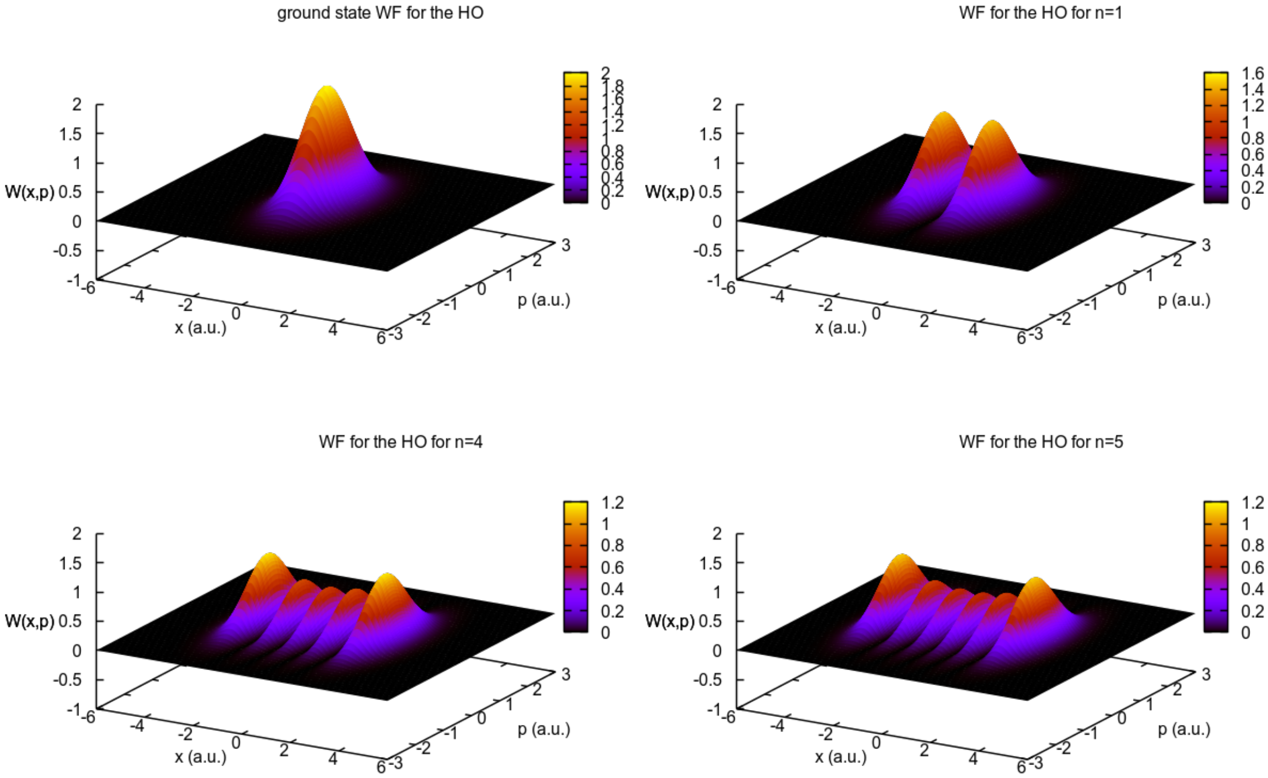

FIGURE 3.2: phase space representation of ground state and first excited state, fourth and fifth excited state WF for the HO.

In figure 3.2, phase space representation for a ground state ($n = 0$) and the first excited state ($n = 1$) WF for the HO are plotted. Next plots represents fourth and fifth excited state WF for the HO. For ground state the distribution is positive

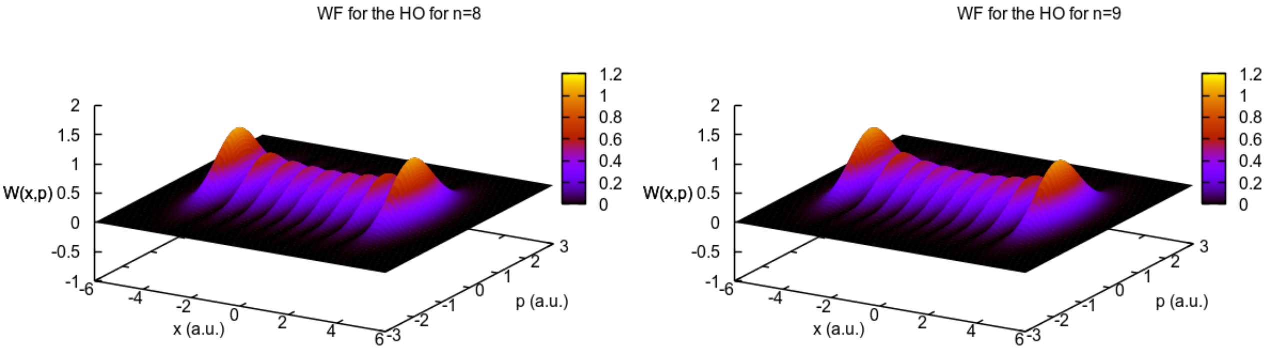

FIGURE 3.3: phase space representation of eighth and ninth excited state WF for the HO.

everywhere but for first excited state the distribution is not strictly positive. Real part of $W(x, p)$ is plotted in all the cases.

In figure 3.3, eighth and ninth excited state WF for the HO are shown. In ground state (n=0), WF is positive everywhere. Whereas, through first and ninth excited state ($n \neq 0$), we find the distribution to be positive as well as negative and the difference between the peaks decreases as n increases. Real part of $W(x, p)$ is plotted in all the cases.

3.1.3 Result and Discussion

- The point where exponential decay goes to zero indicates the 'classical turning point', beyond this point lies the classically forbidden region. The area under the exponentially decaying line is quasiprobability of the non-classical quantum tunneling behaviour.

  Classical turning point is a point at which the systems total energy (E) is equal to the potential energy (V) of the system. If we go past this point, i.e. when $V > E$, such cases are said to be classically forbidden regions, because from purely classical point of view the probability for the system to be in a state where its potential energy is larger that its total energy (alternatively, for system to have negative energy.) is zero.

- Our calculations are not based on WKB approximations. Therefore the outermost peak of the WF for the HO of the stationary states do not coincide with the classical trajectory [1].

- WF offers a formalism equivalent to the formalism offered by the Schr*ö*dinger picture of quantum mechanics. At limits ($\hbar \rightarrow 0$) WF behaves as the probability distribution does in classical physics. This describes a correlation between the classical and quantum mechanics.

- WF helps in visualization of quantum mechanics in phase space distribution. Quantum mechanics in phase space according to the WF resembles classical Hamiltonian mechanics of non-interacting calssical particles [2].

- WF is primarily used to investigate the spectra of molecules and atoms, tunneling effect, and certain quantum correlations. The Quantum mechanical evolution of the WF for a particle in a Harmonic oscillator follows the same dynamics law as the probability density of an ensembles of classical particles in the same potential.

3.2 Wigner Function Calculations using Fourier Transformation

We propose two different ways in which we can compute the Fourier transform with the shift given for the WF of $\pm q/2$. One way to achieve the transformation is by multiplying the HO wavefunction with the diagonalised eigen vectors of the kinetic energy matrix generated using DVR (Appendix A) method [3]. Second method is to multiply the wavefunction with the Fourier grid hamiltonian matrix.

The kinetic energy matrix, denoted by $\mathbf{K}$, generated using the DVR method is in the position basis. When we diagonalize this kinetic energy matrix,

$$\mathbf{K} = \mathbf{U}^{\dagger}\mathbf{E}\mathbf{U} \tag{3.3}$$

The resultant eigenvalue matrix, **E**, is in the momentum basis. Now, when we multiply a wave function which is in the position basis with the unitary matrix U, we get a vector which is in the momentum basis. Thus, the unitary matrices $U^{\dagger}$ and U act similar to a fourier transform. So, based on this idea we are using the DVR kinetic energy eigenvectors for calculating the Wigner Function.

The conclusion to our proposed hypothesis came out to be negative. We were able to produce the shape of the distribution similar to that of the WF but the amplilude of the distrbution did not match the WF for the HO. The reason for the failure of our assumptions is that in the code written for both the cases, there is a dependece on q. Which results in variation in the amplitude with respect to the variation in the grid size of q.

In figure 3.4 we have plotted the wavefunction generated by multiplying the HO wavefunction with the diagonalised eigen vectors of the kinetic energy matrix generated using DVR method w.r.t. position coordinate. We have shown the dependence of the wavefunction on grid size of q. The wavefunction produced using our first method is plotted for the ground state and ninth excited state for $q = 500$, $q = 1000$ and $q = 2000$. We got the similar results when we apply the second method.

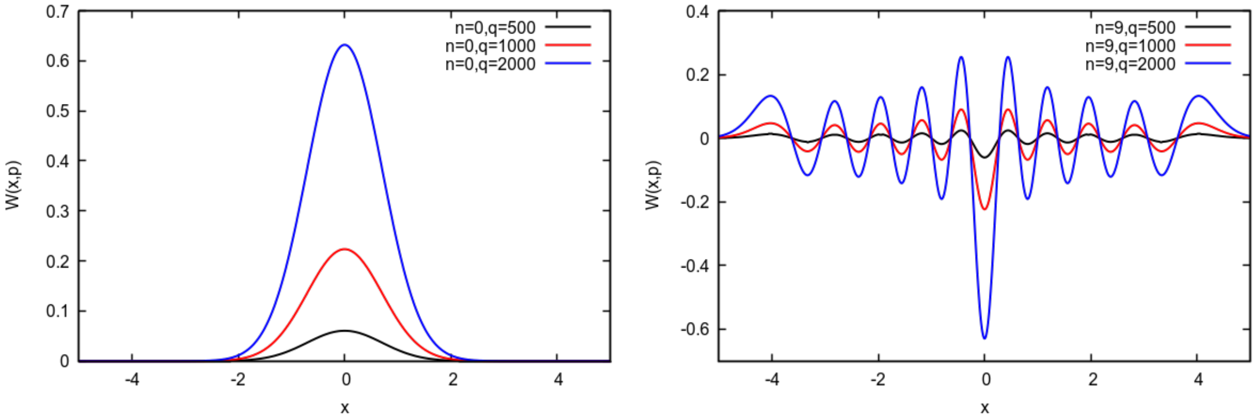

FIGURE 3.4: Ground state and ninth excited state of Wavefunction produced using method one for q=500, q=1000 and q=2000

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Appendix A

Discrete Variable Representation

DVR is a powerful method mostly employed in solving the time-independent Schrödinger equation for a given potential. It is one of the grid-based methods used for obtaining eigenvalues and eigenvectors for a Hamiltonian. In this representation, the associated basis functions are localized about the discrete values of the variables and also the coordinate operators are assumed to be diagonal. DVR has become a versatile tool owing to its simplicity in evaluating kinetic energy matrix elements and the potential operator which requires no integral evaluations and its applications in molecular ro-vibrational spectroscopy and quantum dynamics. Following form of a simple one-dimensional DVR was given by Colbert and Miller[1].

The Kinetic energy operator in one-dimension is given by:

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{d}{dx^2} \tag{A.1}$$

The coordinate 'x' is restricted on the interval (a, b) and the wavefunctions should vanish at the endpoints of the given interval. The grid points $\{x_i\}$ is calculated as:

$$x_i = a + i\frac{(b-a)}{N} \qquad i = 0, 1, 2...., N-1 \tag{A.2}$$

where 'N' is the number of grid points.

The functions associated with a uniform grid as given above are particle-in-a-box

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[1] D.T. Colbert and W.H. Miller, *J. Chem. Phys.* **96**, 1982 (1991).

eigenfunctions:

$$\phi_n(x) = \sqrt{\frac{2}{b-a}} \sin\left[\frac{n\pi(x-a)}{b-a}\right] \tag{A.3}$$

where $n = 1, 2, ..., N-1$. There are only $N-1$ points in the interval and $N-1$ functions as it goes to '0' at the endpoints.

The kinetic energy thus can be represented in its DVR form as given below:

$$\begin{aligned} T_{ij} &= \frac{\hbar^2}{2m}\delta x \sum_{n=1}^{N-1} \phi_n(x_i)\phi_n''(x_j) && \text{(A.4)} \\ &= \frac{\hbar^2}{2m}\left(\frac{\pi}{b-a}\right)^2 \frac{2}{N} \sum_{n=1}^{N-1} n^2 \sin\left(\frac{n\pi i}{N}\right) \sin\left(\frac{n\pi j}{N}\right) && \text{(A.5)} \end{aligned}$$

By summing over all the terms, the reduced form of the kinetic energy term can be written as:

$$T_{ij} = \frac{\hbar^2}{2m}\frac{(-1)^{i-j}}{(b-a)^2}\frac{\pi^2}{2}\left\{\frac{1}{\sin^2[\pi(i-j)/2N]} - \frac{1}{\sin^2[\pi(i+j)/2N]}\right\}, \quad i \neq j \tag{A.6}$$

$$T_{ij} = \frac{\hbar^2}{2m}\frac{1}{(b-a)^2}\frac{\pi^2}{2}\left\{\frac{(2N^2+1)}{3} - \frac{1}{\sin^2(\pi i/N)}\right\}, \quad i = j \tag{A.7}$$

In the interval $(-\infty, \infty)$, the grid spacing 'δx' requires that $N \longrightarrow \infty$. The final matrix representation in this interval is:

$$T_{ij} = \frac{\hbar^2}{2m\delta x^2}(-1)^{i-j} \begin{cases} \pi^2/3\ , & i = j \\ 2/(i-j)^2, & i \neq j \end{cases}$$

where $i = 0, \pm 1, \pm 2, \pm 3, \ldots$.

A sample calculation was done on a model potential of the form:

$$V(x) = e^{-0.1x^2}\left(\frac{x^2}{2} - 0.8\right) \tag{A.8}$$

This potential holds only one bound state with $E = -0.2979596$ *Hartrees*. Given in Figure **??** is a plot of the potential with the bound state.