Strongly Perturbed Harmonic Oscillator

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March 2008

Submitted in accordance with the requirements for the degree of Master of Engineering

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Abstract

The limits of current micro-scale technology is approaching rapidly. As the technology is going toward nano-scale devices, physical phenomena involved are fundamentally different from micro-scale ones [1], [2]. Principles in classical physics are no longer powerful enough to explicate the phenomena involved in nano-scale devices. At this stage, quantum mechanic sheds some light on those topics which cannot be described by classical physics. The primary focus of this research work is the development of an analysis technique for understanding the behavior of strongly perturbed harmonic oscillators.

Developing ‘‘auxiliary’’ boundary value problems we solve monomially perturbed harmonic oscillators. Thereby, we assume monomial terms of arbitrary degree and any finite coefficient desired. The corresponding eigenvalues and eigenvectors can be utilized to solve more complex anharmonic oscillators with non polynomial anharmonicity or numerically defined anharmonicity.

A large number of numerical calculations demonstrate the robustness and feasibility of our technique. Particular attention has been paid to the details as have implemented the underlying formula. We have developed iterative expressions for the involved in-

tegrals and the introduced ‘‘Universal Functions.’’ The latter are applications and adaptations of a concept which was developed in 1990’s to accelerate computations in the Boundary Element Method.

Declaration

I certify that except where due acknowledgement has been made, the work is that of the author alone; the work has not been submitted previously, in whole or in part, to qualify for any other academic award; the content of the thesis is the result of work which has been carried out since the official commencement date of the approved research program; and, any editorial work, paid or unpaid, carried out by a third party is acknowledged.

PANTEA PEIDAEE

31/03/2008

Acknowledgements

I would like to acknowledge the following contributions for the completion of my thesis.

- My supervisor Professor Alireza Baghai-Wadji for his direct support,
- Partial support provided by the Victorian Partnership for Advanced Computing (VPAC), Australia,
- RMIT Library for providing valuable books,
- My family and my colleagues, Amirabbas Rezaee, Istiaque Ahmed, and Rosmiwati Mohd Mokhtar, for their moral and technical support through out the period of this research.

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h	Planck constant
$\hbar$	Reduced Plank Constant ($h/2\pi$)
x	Spatial Coordinate
ξ	$\xi = \sqrt{\alpha}x$, Reduced Spatial Coordinate
m_0	Electron Mass
δ_{mn}	Kronecker Delta Symbol
a	Annihilation Operator
$a^\dagger$	Creation Operator
$\varphi(x)$	Eigen Function in x domain
$\psi(\xi)$	Eigen Function in ξ domain
$\widetilde{\psi}(\xi)$	Perturbed Eigen Function in ξ domain
E	Eigen Value
$\widehat{E}$	Normalized Eigen Value
$\widetilde{E}$	Perturbed Eigen Value
$\widetilde{\widehat{E}}$	Perturbed Normalized Eigen Value

Chapter 1

Introduction

1.1 Motivation

The limit of current micro-scale technologies urge scientists and researchers to anticipate the development of the nano-scale devices. In doing research in this field of study, quantum mechanics is the most crucial branch of theoretical physics with vast applications in practical physics which avoids deficiencies of classical physics at atomic and subatomic level.

Quantum, meaning how much in Latin, refers to discrete units that in quantum theory assigns to energy of an atom in stable or equilibrium state. The discovery of the fact that waves can be assumed as a small packet of energy which is called quanta led to the introduction of quantum mechanics.

The basic idea that led to the discovery of quantum mechanics was the study of light which is an electromagnetic wave. This initialized an explanation for the spectra of light emitted by different type of atoms. Originally, it was providing justification for

electron's residing in its orbital, which cannot be explained by classical mechanics. When in 1900 Max Planck found that the energy of waves are quanta, Einstein utilized this revolutionary finding to illustrate that electromagnetic waves such as light consist of elementary particle called photon. Each photon has discrete energy level which directly depends on the frequency of the wave.

The precursor of the modern theory is the first twenty-five years of quantum mechanics [3]. The first quarter of the twentieth century was a golden era for advancement in quantum mechanic. Scientists including Heisenberg, Planck, de Broglie, Bohr, Schrödinger, Dirac, Einstein and others had great contribution in establishing and promoting quantum mechanics [3], [4]. The creation of quantum mechanics provides us with a theory that appears to be in complete accordance to our empirical knowledge of all nonrelativistic phenomena [5].

Quantum mechanics is a more fundamental concept than Newtonian classical mechanics. It explains those phenomena which are in small scale level and classical mechanics cannot have any explanation for the observed phenomena. For instance, from Newtonian point of view an electron in an atom should move toward nucleus and crash into it. In contrast to the classical picture, electron is moving in an orbit around the nucleus.

In quantum mechanic, formulating state of the system at any time is defined by a complex-valued wave function. From the mathematical point of view, the fact that the probability of finding an electron at a particular time and region around the nucleus can be obtained is in contrast to classical mechanics that could not calculate prediction

of conjugate variables such as momentum and position (in one direction) simultaneously. In fact, electron is always considered to be located somewhere in the space with unknown but accurate position. The contours of constant probabilities will enable us to conceptualize a cloud around the nucleus of atom. This cloud is the most probable place where the electron might be located. In Heisenberg's uncertainty principle, inability to accurately locating a particle is expressed.

Generally speaking, quantum mechanics can explain four types of phenomena that classical mechanics cannot explain:

- ⋆ Discretization of certain physical quantities
- ⋆ Uncertainty principle
- ⋆ Quantum entanglement
- ⋆ Wave particle duality

Quantum mechanics has tremendous success in describing many features of our world [57]. Chiefly, it has a logical justification for phenomena at atomic and subatomic levels that classical mechanics was not able to explain them. In chemistry, it has a great impact on clarification of atoms combined covalently to form a molecule. It gives us a quantitative approximation that how much molecules are vigorously favorable to each other.

Most of our contemporary technology is operating on a scale which has significant quantum impact. For instance, laser, electron, microscope and transistor are significantly

influenced by quantum effects. Transistors are semiconductor-based microelectronic devices the study of which led to their invention along with diodes [57].

Researchers are moving toward manipulation of quantum states. The effort resulted in the development of a secure broadcasting of information by quantum cryptography. One of the ultimate goals is construction of quantum computers in order to work exponentially faster than the current ones in computational tasks. Quantum teleportation which allow transmission of quantum states over arbitrary distances is one of the hot spots in quantum mechanics [18].

All the above-mentioned facts and reasoning, along with the remaining significance of the theoretical findings and probable suggestion of a unified methodology for a robust computational analysis of perturbed systems had motivated me and had an impact on my taking up of this research.

1.2 Objective

The main objective of my research is to carry out theoretical and numerical computational work on canonical and perturbed harmonic oscillators. Our target is to devise a methodology that provides robust numerical calculations of eigenpairs for perturbed oscillators with a flexible range of perturbation and simultaneously eliminates the cumbersome load of traditional computations.

We pose our ‘‘original’’ (given) problem as a complicated problem, which in our case is a strongly perturbed harmonic oscillator. Our imposed perturbation is an arbitrary

monomial potential function added to the parabolic potential of harmonic oscillator. As is shown in this work the analysis can be extended to include polynomial perturbations. Eigenvalues and the corresponding eigenfunctions for a variety of perturbed harmonic oscillator have been calculated and presented in this work.

Our method consists of the construction of an auxiliary problem. An auxiliary problem, as used in our formulations is a boundary value which is related to our original (given) problem but has a simpler structure to the effect that its eigenpairs can be calculated comparatively straight forwardly analytically or numerically [56]. Here, the main characteristic of our auxiliary problem that urge us to choose it as our gauging problem, is the fact that we can obtain its eigen solutions in closed-form. Therefore, we start our analysis by finding out the solutions of the unperturbed harmonic oscillator. More broadly speaking, closed-form solutions are equations which are utilized to solve given problems in terms of mathematical operators and functions from a given generally accepted set.

We considered the perturbation of our system as a monomial with a general form, which means that it can have any arbitrary power and coefficient. Therefore, our assumption includes linear, quadratic and other higher-order monomial perturbations. We set up the wave function of the perturbed system as a linear combination (superposition) of the original eigensolutions. This is permitted since the eigenfunctions of the harmonic oscillator constitute a complete set of orthonormal functions which can serve as basis. As the next we carry out the ‘‘action’’ of the original system on the auxiliary system and vice versa. Then, we subtract the two ‘‘actions’’ and minimize the weighted resulting

residual ‘‘action’’ by using the orthonormal functions of the harmonic oscillator.

Thereby, we have implemented our own method for the calculation of the involved integrals. Subsequently the eigenpairs of the original problems are calculated. As has been outlined in this work our method can straightforwardly be extended to solve polynomial perturbations of any complexity and order. An interesting feature of out technique is that the involved interaction matrix associated with each monomial can be precalculated separately (individually) and stored. As it is shown in an upcoming publication this procedure is amenable to symbolic computation and further generalized our concept of the Universal Functions utilized in this thesis.

1.3 Summary of Chapters

In Chapter 2, aspects of the quantum mechanics relevant to this work have been reviewed. Then, basic ideas needed for understanding the problems solved in the following chapters are discussed. In this research, the solution of the harmonic oscillator are used as analysis tools. Therefore, the definition of the harmonic oscillator is crucial and will be discussed in this chapter. Two different conceptions for harmonic oscillator will be explained separately. The first one is the classical concept which can be discussed based on the classical or Newtonian mechanics principles. The classical view concern systems in which the displacement of a mass point from its equilibrium will introduce a restoring force to the mass (such as spring or a pendulum). Quantum harmonic oscillator is different from classical harmonic oscillator in the aspect that this system can not be explained by the tools developed in classical mechanics. Quantum harmonic

oscillator can be formulated by quantum mechanics rather than its analogous, classical mechanics.

The involved notations are described very briefly in Chapter 2. I describe Hermite polynomials, as they play a significant role in the formulation of simple harmonic oscillator. Moreover, I talk about eigenvalues, eigenvectors and eigenvalue problems due to the fact that I use these terms very often in my thesis.

In literature review of Chapter 3, we discuss the traditional (standard) way of formulating changes in harmonic oscillator when a linear perturbation is introduced.

In Chapters 4 and 5, I used the notation of Hamiltonian operators which is utilized in order to find the kinetic and potential energies of a moving particle. These two chapters are based on early formulation of our theory reported in two papers published in ACES 2007 (Applied Computation Electromagnetics Society) and PIERS 2007 (Progress In Electromagnetics Research Symposium) [6], [7].

Chapter 4 is the ‘‘heart’’ of the thesis and details the implementation of the concept of auxiliary problems and Universal Functions. We propose an easy-to-implement method for the calculation of eigenfunctions of monomially perturbed harmonic oscillator. Our method is based upon using the eigensolutions of the unperturbed harmonic oscillator as auxiliary gauging functions. The obtained eigenfunctions of perturbed harmonic oscillator can be used as complete set of functions for analyzing related boundary value problems.

This technique with appropriate variations has successfully been applied to a variety

of related boundary value problems, [8], [9], [10], and [11].

We present our approach for solving any monomial perturbation added to harmonic oscillator which among others may include linear perturbation. We consider the idea based on the construction of an auxiliary boundary value problem to be original and promises applications for beyond the work presented here.

In Chapter 5 numerical results of the calculated eigenfunctions of monomially perturbed harmonic oscillators are presented and compared with the corresponding solutions of the (unperturbed) solutions of the harmonic oscillator. Varies solutions depending on the degree of the monomials and the ‘‘strength’’ of the perturbation are presented. The continuous variation of the perturbed solutions by increasing the perturbation is encouraging. The orthonormality property of the obtained solutions validates our concept.

In Chapter 6 prospect for the future work are outlined.

In Chapter 7 the summary of our achievement along with conclusions of my thesis are given.

Chapter 2

Background

2.1 Introduction

At first glance, this thesis may strike you as excessively mathematical [12]. You may ask whether this much of explanation and mathematics is a real necessity? I would say may be not but physics is like carpentry. By using the right tool your job would become much easier [12].

In this Chapter, I am going to explain the basics. The first topic that I am going to discuss is the history and the nature of quantum mechanics. The discussion is on how it started.

After this brief introduction on quantum mechanic, I will focus on explaining the harmonic oscillator due to the fact that this thesis is reformulating the changes in characteristics of harmonic oscillator such as its eigenvalues. Then, several fundamental terms which are implemented in my formulation and the solution of the problem will be introduced with a brief clarification of the involved notions. Due to the fact

that we set up the Schrödinger equation for the unperturbed and perturbed harmonic oscillators and by solving that equation eigenvectors and eigenvalues of the canonical and perturbed problem can be obtained, we discuss all those terms such as, Schrödinger equation, eigensolution and so on with their properties in order to shed light on this vital fact of quantum mechanics.

Subsequently, alternative views for solving perturbed harmonic oscillator found in literature have been described.

2.2 Quantum Mechanics: A Brief Review of the Concepts Used

By the end of nineteen century and after nearly 200 years, classical Newtonian mechanics was still the basis of theoretical explanation of any physical or chemical phenomena. In classical mechanics motion of electron assumes propagation of electron in wave format. Therefore, based on that view if there is an obstacle which has higher energy level than the electron (e.g. potential well), the electron cannot pass through the wall. In contrast, in quantum mechanics electron is counted as a packet of energy, and formulated such that, it can penetrate the barrier exponentially decreasing through that potential. It was generally believed that all natural phenomena are well established and well behaved, due to the fact that they could be described by classical motion of electrons. It was unimaginable for them to foresee that the following decades will revolutionize theoretical physics and classical mechanics no longer will use to describe electrons motion [43]. First, some shades of doubt were introduced by the work of

Lorentz, Einstein and others that high speed phenomena could not be described in the category of classical mechanics.

Different line of thought which was commenced by Planck, Heisenberg, Schrödinger and others, led to the realization that classical Newtonian mechanics fails to elucidate atomic phenomena. When you search through the quantum mechanic books, you instantly will notice that Planck was the pioneer of quantum mechanics [3], [13].

The birth of quantum mechanics to the universe is on fall of 1900. The day when, the German Physicist, Max Planck presented two papers at the German Physicist Society [3]. These two papers were presented on October 19 and December 14 of 1900. These papers have had that much revolutionary impact that science historians can not concur as which of these two papers should be considered as a true start [44].

Those papers were final analysis of the energy distribution in what Planck called normal spectrum. He discovered that the energy of waves can be explained as consisting of small packets or quanta. Later, Albert Einstein utilized Planck's idea to illustrate that electromagnetic waves such as light consists of particles called photon with a discrete energy level depending on frequency [45].

2.3 Harmonic Oscillator

Harmonic oscillator played a significant role in the theoretical advancement at the beginning of this century, since it was an indispensable part of many of the theories which led to quantum mechanics. Any system which is fluctuated by a small amount

near a configured equilibrium can be modelled either by harmonic oscillator or by a collection of decoupled harmonic oscillators [44]. Since the dynamic complexity of a collection of decoupled harmonic oscillator is not more than that of a single one, in tackling the problems we imagine the general form. In fact, harmonic oscillator was often regarded as a beginning point of theories which involves electronic movement in atoms, molecules or crystals. It became known that an atom consisted of a nucleus and certain number of electron which are moving around the nucleus [46].

In classical mechanics, harmonic oscillator is a system in which, when any disturbance that displaces it from its equilibrium occurred, experiences a restoring force, F, proportional to the displacement x according to Hooke's law [47].

In one dimension, a harmonic oscillator is a particle with mass m, oscillating back and forth around the zero point or origin 0 (equilibrium). It should be pointed out that this displacement always tends to move back to the origin point of 0.

In my research, I assume a simple harmonic oscillator which means that it does not have a driving force or friction force.

$$F = -kx \tag{2.1}$$

Since any conservative field $F(x)$ can be written as the negative gradient of a potential function $V(x)$, $F = -dV/dx$, the potential energy of the particle can be found by integrating F, which is the following:

$$V(x) = \frac{1}{2}kx^2 \tag{2.2}$$

The following Hamiltonian of the one dimensional harmonic oscillator will have a potential of zero at the origin, that is, $V = 0$ when $x = 0$.

$$H(x, p) = -\frac{p^2}{2m_0} + \frac{kx^2}{2} \tag{2.3}$$

It drives from Hamiltonian's equations of motions in which the conjugate variables x and p are determined by the equations:

$$\frac{\partial x}{\partial t} = \frac{p}{m_0} \tag{2.4}$$

and

$$\frac{\partial p}{\partial t} = -kx. \tag{2.5}$$

By taking the derivative of the equation (2.4) with respect to t and then replacing $\partial p/\partial t$ by the equation (2.5), we obtain

$$\frac{\partial^2 x}{\partial t^2} = -\frac{k}{m_0}x. \tag{2.6}$$

It is customary to introduce the angular frequency

$$\omega = \left(\frac{k}{m_0}\right)^{1/2}. \tag{2.7}$$

Therefore, by substituting equation (2.7) into (2.6), we obtain

$$\ddot{x} + \omega^2 x = 0. \tag{2.8}$$

Here, the dot symbolizes the derivative with respect to time. The solutions of this homogenous ordinary differential equation are:

$$x = C\, e^{\pm i\omega t}. \tag{2.9}$$

Hence, the general solution for harmonic oscillator is

$$x = Ae^{i\omega t} + Be^{-i\omega t} \tag{2.10}$$

With the two unknown parameters A and B which have to determined from initial conditions. By setting the condition that the value of the solution at zero point (the origin of our coordinate system) is zero, that is, $x(0) = 0$, we can obtain the solution

$$x(t) = A \sin \omega t. \tag{2.11}$$

The motion of harmonic oscillator depends on two parameters:

ω: the angular frequency,

and

A: the amplitude of oscillator.

$$\omega = 2\pi\gamma. \tag{2.12}$$

In which γ is the frequency of oscillator or the number of complete cycles covered per unit time. By replacing the equations (2.12) and (2.11) into the equation (2.4), the following result is obtained:

$$p(t) = A\, m_0\, \omega\, \cos\omega t \tag{2.13}$$

By plugging the equations (2.11) and (2.13) into equation (2.3), we will get the following result;

$$E = H(x,p) \tag{2.14a}$$

$$= \frac{1}{2}\, m_0\, A^2\omega^2 \tag{2.14b}$$

Energy is a function of ω when m and A are constant. Due to the fact that ω is squared, it can be said that the values of ω^2 and respectively (the total energy) E are always positive. For more detail refer to [4], [14] and [15].

2.4 Quantum Harmonic Oscillator

Quantum harmonic oscillator is one of the most fascinating mechanism and is one of the most significant intellectual achievement of twentieth century [42]. In quantum mechanics harmonic oscillator is defined as the vibration of a diatomic molecule for the fact that is somewhat like that of two masses on a spring with a potential energy that depends on the square of displacement from the equilibrium state. As it turns out, the energy levels of harmonic oscillator are quantized at equally spaced values.

The most astonishing difference between simple and quantum harmonic oscillator is the so-called zero-point vibration of the $n = 0$ ground state. This statement means that unlike simple harmonic oscillator molecules are not completely at steady state, even at absolute zero temperature.

The quantum harmonic oscillator has far more inference than the simple diatomic molecule. It serve as a fundamental concept for the elucidation of other problems such as complex modes of vibration in larger molecules, the motion of atoms in a solid lattice, and the theory of heat capacity. In real systems, energy quantization is equal only for the lowest levels in which the potential is an excellent approximation of the mass on a spring type harmonic potential. The anharmonic terms which emerge from the potential of a diatomic molecule are valuable for plotting the detailed potential of such systems.

In order to obtain a solution to the Schrödinger equation and to appreciate the peculiarities of nature at quantum level, I proceed with a simple form of problem. Assuming

the wave function $\psi(x)$ and potential $V(x)$ depend on the x-coordinate only. Then, the corresponding Schrödinger equation for one-dimensional problem is an Ordinary Differential Equation (ODE):

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{2.15}$$

This equation can be solved for various special forms of the potential $V(x)$. In this thesis, we have taken $V(x)$ to represent any monomial of the from αx^r added to a parabolic potential. In particular for $\alpha = 0$ we obtain the ideal harmonic oscillator characterized by the potential:

$$V(x) = \frac{1}{2}\, m_0\, \omega^2\, x^2 \tag{2.16a}$$

$$= \frac{1}{2} k x^2 \tag{2.16b}$$

In the above equation ω is the angular frequency of the harmonic oscillator.

2.5 Hermite Polynomials

From mathematical point of view, Hermite polynomials are classical orthogonal polynomials originate from the theory of probability. They are the eigenstates of the quantum harmonic oscillator. The name of the Hermite polynomial is for the honour of Charles Hermite. He was a French mathematician who did research on number theory, orthogonal polynomials, quadratic forms and etc. Hermitian operators are named after him

as well. He was the first scientist who proved that e is a transcendental number. Later on, Lindemann by using his methodology proved that π is transcendental [53].

Hermite polynomials can be defined in different ways. These definitions are not completely the same; based on the properties that each definition may have, they are used in different fields of knowledge.

General form:

$$H_n(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2} \tag{2.17}$$

Physicists notation:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \tag{2.18}$$

Probabilists notation:

$$H_n(x) = 2^{n/2} H_n^{\text{prob}}(\sqrt{2x}) \tag{2.19}$$

Equation (4.13a) is most widely used form. Probabilists notation often follow the general form, due to the fact that the function

$$\frac{1}{\sqrt{2\pi}} e^{-x^2/2} \tag{2.20}$$

is the probability density function for the normal distribution. The standard deviation and expected value of this function are, respectively, 1 and 0.

The first six Hermite polynomials based on the probabilists view are as follows:

$$
\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= x \\
H_2(x) &= x^2 - 1 \\
H_3(x) &= x^3 - 3x \\
H_4(x) &= x^4 - 6x^2 + 3 \\
H_5(x) &= x^5 - 10x^3 + 15x \\
H_6(x) &= x^6 - 15x^4 + 45x^2 - 15
\end{aligned}
$$

The followings are the first eleven Hermite polynomials $(H_0, \cdots, H_{10})$ based on physicist's definition of Hermite polynomials. This definition has been used for solving the problems in this thesis.

$$H_0(x) = 1 \tag{2.21a}$$

$$H_1(x) = 2x \tag{2.21b}$$

$$H_2(x) = 4x^2 - 2 \tag{2.21c}$$

$$H_3(x) = 8x^3 - 12x \tag{2.21d}$$

$$H_4(x) = 16x^4 - 48x^2 + 12 \tag{2.21e}$$

$$H_5(x) = 32x^5 - 160x^3 + 120x \tag{2.21f}$$

$$H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120 \tag{2.21g}$$

$$H_7(x) = 128x^7 - 1344x^5 + 3360x^3 - 1680x \tag{2.21h}$$

$$H_8(x) = 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680 \tag{2.21i}$$

$$H_9(x) = 512x^9 - 9216x^7 + 48384x^5 - 80640x^3 + 30240x \tag{2.21j}$$

$$H_{10}(x) = 1024x^{10} - 23040x^8 + 161280x^6 - 403200x^4 + 302400x^2 - 30240 \tag{2.21k}$$

In the following typical graphs of Hermite polynomials have been shown:

The above graph is the second solution of Hermite polynomials ($H_2(x)$) which has the following form:

$$H_2(x) = 4x^2 - 2 \tag{2.22}$$

This is $H_3(x)$. However, due to the fact that Hermite Polynomials start from H_0 , this graph is for:

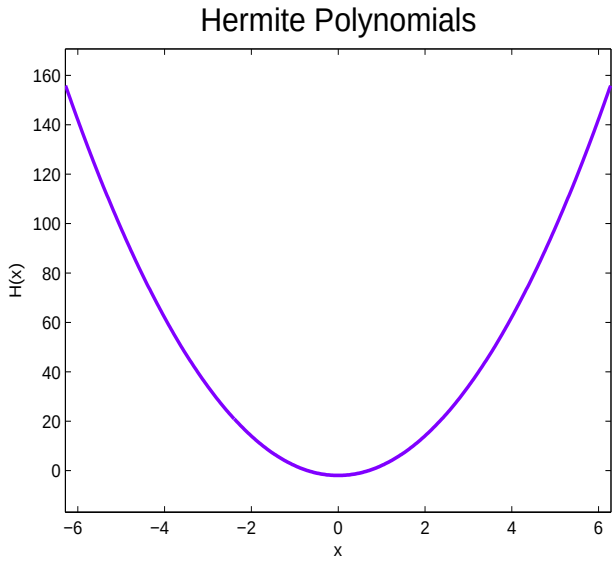

Figure 2.1: The graph of 2nd Hermite Polynomial

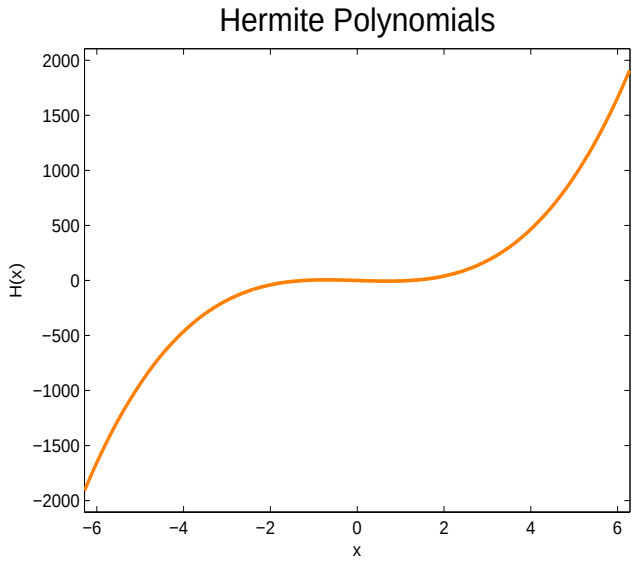

Figure 2.2: The graph of 3rd Hermite Polynomial

$$H_3(x) = 8x^3 - 12x \tag{2.23}$$

This figure shows the first five solutions of Hermite polynomials presented together. In this figure when n=0, Hermite polynomial is $H_0(x) = 1$. The next curve is $H_1(x) = 2x$,

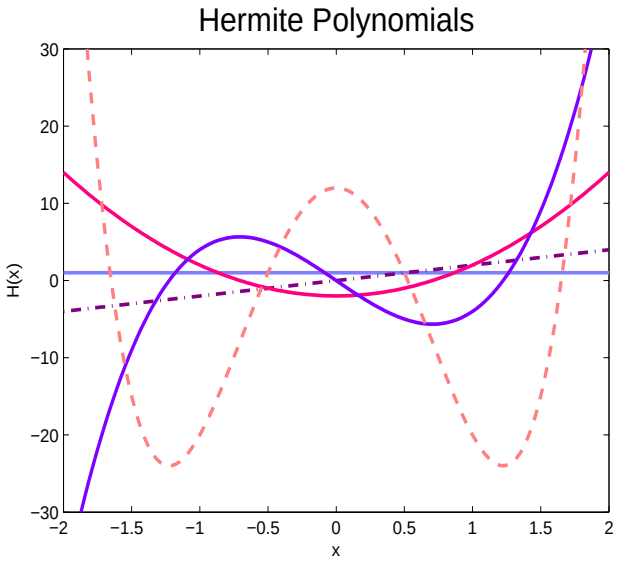

Figure 2.3: The first five Hermite Polynomials

the blue line having the slope of 2. Dotted line corresponds to $H_2(x) = 4x^2 - 2$. As the number of n increases, the power of x increases in Hermite polynomials. The long dotted form stands for $H_3(x) = 8x^3 - 12x$. The purple one is for $H_4(x) = 16x^4 - 48x^2 + 12$.

Hermite polynomials have desirable properties which will be summerised here. The first and the most notable property of Hermite polynomials is the orthogonality. $H_n(x)$ for $n \in N$ are n^{th}-degree polynomials that are orthogonal to each other with respect to the weight function explained below.

Weighting functions for probabilists and physicists are defined as $e^{-x^2/2}$ and e^{-x^2}, respectively.

As a result of the orthogonality we can show that from physicist's point of view:

$$\int_{-\infty}^{\infty} dx\, H_n(x) H_m(x)\, e^{-x^2} = n!\, 2^n \sqrt{\pi}\, \delta_{nm} \tag{2.24}$$

This is the representation for the orthogonality of Hermite polynomials. Thereby, δ_{nm} stands for Kronecker's symbol. It is 1 when $n = m$, and is 0 otherwise. Further important properties of Hermite polynomials are summarized below [16], [17].

2.5.1 Hermite's Differential Equation

Hermite polynomials $H_n(x)$ $(n \in N)$ satisfy the following differential equation:

$$H_n^{''}(x) - 2x\, H_n^{'}(x) + 2nH_n(x) = 0 \tag{2.25}$$

Here, the prime symbolizes the derivative with respect to the independent spatial coordinate x.

2.5.2 Hermite's Recursion Relation

Hermite polynomials also satisfy the following recursion formula:

$$H_{n+1}(x) = 2x\, H_n(x) - H_n^{'}(x) \tag{2.26}$$

2.5.3 Hermite's Recurrence Relation

In addition the $(n+1)^{\text{th}}$ Hermite polynomial satisfies the following relation with its two immediate predecessor polynomials:

$$H_{n+1}(x) = 2x\, H_n(x) - 2n\, H_{n-1}(x) \tag{2.27}$$

2.5.4 Hermite's Generating Function

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(x)\, t^n$$

2.5.5 Hermite's Expected Value

From probabilists point of view, assume x is a random variable with a normal distribution and standard deviation of unity with expected value of μ, under these conditions the following important result for the expected value of $H_n(x)$ holds true:

$$E\left(H_n(x)\right) = \mu^n \tag{2.28}$$

2.5.6 Hermite Polynomial Application

Utilizing the Hermite polynomials from the physicist's prospective, we define the wave function $\psi_n(x)$ as follows:

$$\psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\, n!\, 2^n}} e^{-x^2/2} H_n(x) \tag{2.29}$$

The wave functions $\psi_n(x)$ involve the square root of the weight function $e^{-x^2/2}$ and also have been properly scaled to yield:

$$\int_{-\infty}^{\infty} dx\, \psi_n(x)\, \psi_m(x) = \delta_{nm} \tag{2.30}$$

Hermite functions also satisfy the differential equation which is,

$$\psi_n''(x) + \left(2n + 1 - x^2\right)\, \psi_n(x) = 0 \tag{2.31}$$

The above equation corresponds to the Schrödinger equation for harmonic oscillators in quantum mechanics. Therefore, Hermite functions are eigenfunctions of the Schrödinger equation for harmonic oscillator.

2.6 Schrödinger Equation

Schrödinger equation was first proposed by the Austrian Physicist, Erwin Schrödinger in 1925. The theoretical and experimental rationalization of the Schrödinger equation inspired the discovery of the Schrödinger equation. Schrödinger equation describes the motion of non-reletivistic particles. This equation explains the space- and time-dependence of quantum mechanical systems (time-dependent Schrödinger equation). Schrödinger equation is the fundamental equation of (non-relativistic) quantum mechanics, playing a role similar to Newton's law in classical mechanics [48].

From a mathematical point of view every quantum mechanical system is associated with a complex Hilbert space. Therefore, every state of the system is illustrated by a unit vector in that space. The state vector determines the probabilities for the outcome of all possible measurements practical to the system. Since the state of a system generally changes over the time, that is, the state vector is time dependent, Schrödinger equation

provides a quantitative rate of changes of the state vector involving the Hamiltonian of the system:

The Hamiltonian of the system as it is derived from the classical Hamiltonian with a possible correction term for relativity.

$$\hat{H}\psi = i\,\hbar\,\frac{\partial}{\partial t}\psi \tag{2.32}$$

For many of the real-world problem Hamiltonian is not a time-dependant energy operator. Based on this observation, it can be said that time-independent Schrödinger equation is simplified form of time-dependant Schrödinger equation. The one-dimensional time-independent Schrödinger equation for a particle can be written as

$$-\frac{\hbar^2}{2m_0}\,\frac{d^2}{dx^2}\,\psi(x) + V(x)\psi(x) = E\psi(x), \tag{2.33}$$

where m is mass of the particle and $V(x)$ is the potential that particle moves in.

Likewise, three-dimensional time-independent Schrödinger equation can be written as

$$-\frac{\hbar^2}{2m_0}\,\nabla^2\,\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z) \tag{2.34}$$

In which the second derivative has been replaced by nabla operator ∇^2.

A time-independent Hamiltonian operator is associated with a set of quantum states which are known as energy eigenstates.

For relatively simple cases, solutions of time-independent Schrödinger equation can be obtained in closed-form. These solutions provide insight into the nature of quantum phenomena under consideration.

Moreover, they may provide a reasonable approximations of behaviour of more complex systems. For instance, in quantum mechanics, molecular vibrations can be reasonably well modelled as harmonic oscillators.

2.7 Schrödinger Equation for Harmonic Oscillator

By using the classical ideal spring potential, we can obtain the Schrödinger Equation for harmonic oscillator:

$$V(x) = \frac{1}{2}\,k\,x^2 \tag{2.35a}$$

$$= \frac{1}{2} m_0\,\omega^2\,x^2 \tag{2.35b}$$

In which $\omega = \sqrt{k/m_0}$ is the angular frequency and in $\omega = 2\,\pi\nu$, ν is the frequency.

In order to simplify our discussion, we assume that V and ψ only depend on x. Then, the Schrödinger equation corresponding to this one dimensional problem can be written as

$$-\frac{\hbar^2}{2m_0}\,\frac{d^2}{dx^2}\,\psi(x) + V(x)\psi(x) = E\psi(x), \tag{2.36}$$

where it potential energy is equation(2.35a) ; therefore, the so-called Schrödinger equation for harmonic oscillator is

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\psi(x) + kx^2\psi(x) = E\psi(x) \tag{2.37}$$

2.8 Hermitian Operators

In simple words, Hermitian is the name of self-adjoint in physics literature. Self-adjoint operator is the one that its adjoint's matrix is Hermitian on a finite-dimensional inner product space. The conjugate transpose of a Hermitian matrix is equal to itself. Utilizing the finite-dimensional spectral theorem, Hermitian operators can be shown to be represented by a diagonal matrix with real numbers.

Hermitian operators are used in quantum mechanics. In Dirac's formulation of quantum mechanics, physical observables such as position, momentum, angular momentum and spin are represented by Hermitian operators on a Hilbert space [51], [52].

The most important Hamiltonian operators is the following which as an observable corresponds to the total energy of a particle of mass m and has a potential of V:

$$H\Psi = -\frac{\hbar^2}{2m_0}\nabla\Psi + V\Psi \tag{2.38}$$

A partially defined linear operator A is called symmetric when it has the following property on Hilbert space H, which is a real or complex vector with a positive-definite Hermitian form that is complete under its norm,

$$\langle Ax|y\rangle = \langle Ay|x\rangle \tag{2.39}$$

For all elements of x and y in A domain. Based on the Hellinger-Toeplitz theorem, an everywhere defined symmetric operator is bounded. Bounded symmetric operator is called Hermitian operator.

In other words, generally linear operators are complex quantities which mean that their correspondence to dynamical variable would be complex. On the other hand, physical quantities like momentum and position when they are measured are real numbers. As a result of that, the linear operators that represent dynamical variables must be a real linear operator. Such operators are defined as follows and are called Hermitian operators:

$$|q\rangle = L|p\rangle \tag{2.40}$$

When L is a linear operator and the bra ($\langle q|$) associated with the ket ($|q\rangle$) can be written:

$$\langle q| = \langle p|L^\dagger \tag{2.41a}$$

$$\begin{aligned} \langle q| &= (L|p\rangle)^\dagger \\ &= (|q\rangle)^\dagger \end{aligned} \tag{2.41b}$$

Here, $L^\dagger$ is the Hermitian adjoint of L. The bra $\langle q|$ as it is shown is the Hermitian

adjoint of $\big|q\rangle$. Therefore, it can be said that this is the result of a linear operator like $L^\dagger$ operating on $\langle p|$. It is immediate to show that

$$L^{\dagger\dagger} = L. \tag{2.42}$$

We have

$$\big|a\rangle = L\big|p\rangle. \tag{2.43}$$

Where $\big|p\rangle$ is an arbitrary ket vector. Its associated bra is

$$\langle a\big| = \langle p\big|L^\dagger. \tag{2.44}$$

If we take one more step and take adjoint again, we have

$$\big|a\rangle = L^{\dagger\dagger}\big|p\rangle. \tag{2.45}$$

If we take the scalar product of the equation (2.45) with an arbitrary bra $\langle c\big|$ and replace the right-hand side by the equation (2.43), we obtain

$$\langle c\big|a\rangle = \langle c\big|L^{\dagger\dagger}\big|p\rangle \tag{2.46a}$$

$$\langle c\big|L\big|p\rangle = \langle c\big|L^{\dagger\dagger}\big|p\rangle \tag{2.46b}$$

Since $\langle c\big|$ and $\big|p\rangle$ are arbitrary. Consequently, $L^{\dagger\dagger} = L$ is proven. In addition, if we let $\big|c\rangle = L\big|p\rangle$ and $\langle c\big| = \langle p\big|L^{\dagger}$, we have

$$\langle p\big|L^{\dagger}\big|c\rangle = \langle c\big|L\big|p\rangle^{*}. \tag{2.47}$$

If the linear operator is self-adjoint, it means that $L^{\dagger} = L$ we obtain

$$\langle p\big|L\big|c\rangle = \langle c\big|L\big|p\rangle^{*} \tag{2.48}$$

As mentioned earlier, the outcome of a measurement is a real number. This property has been significant in formulating the theory in this thesis. The fact that this measurement is coming from the expectation value of $\langle Q\rangle = \int dr\psi^{*}\hat{Q}\psi$ will impose some restriction on dynamical variables Q. Let's say

$$\langle Q\rangle = \langle Q\rangle^{*} \tag{2.49}$$

We have,

$$\int dr\psi^{*}\hat{Q}\psi = \int dr(\psi\hat{Q})^{*}\psi \tag{2.50}$$

In general this integration extends over all the coordinates of all participating particles. For instance, if we have n particles, we have 3 coordinates for each particle which result in $3n$ coordinates. If we include spin, then another integration has to be carry out over

the spin variables as well. Consequently, it will be $4n$ if spin is included [53]. In this way we will save in writing and instead of saying the details we remove dr and write the integral in the following form;

$$\langle Q \rangle = \int \psi^* \hat{Q} \psi \tag{2.51}$$

and

$$\int \psi^* \hat{Q} \psi = \int (\hat{Q}\psi)^* \psi \tag{2.52}$$

The above formula shows that integrated and summed over all the coordinates of particles which constitute the system. It is worth mentioning that operators satisfying (2.52) were first studied by Charles Hermite.

2.9 Eigenvalues and Eigenvectors of Hermitian Operators

In general, the act of a hermitian operator on a vector will change the magnitude or direction of the vector. If we imagine that the action of a hermitian operator on a vector will change the magnitude of that vector, it means that the magnitude of that vector is multiplied by a constant. We can write

$$\hat{A}\big|a_i\rangle = a_i\big|a_i\rangle \tag{2.53}$$

When A is the operator and $\left|a_i\right\rangle$ is the vector. The subscript shows that N independent vectors satisfy this equality. Constants a; and vectors $\left|a_i\right\rangle$ $(i = 1, \cdots, N)$ which satisfy (2.53) are referred to as the eigenvalue and the corresponding eigenvectors of operator $\hat{A}$.

In German language ‘‘eigen’’ means ‘‘self’’, ‘‘characteristic’’. Therefore, the eigenvectors and eigenvalues are characteristic (characterizing) vectors and values of the operator. The set of eigenvalues is customarily called the spectrum of the operator.

2.10 Eigenvalue Problems

The classical view suggests that the eigenvalue problem can be defined as followings:

$$Av_n = \lambda_n v_n \qquad n = 1, \cdots, N \tag{2.54}$$

Here, we assume A to be a real and also symmetric matrix. On the other hand, A might be singular and the eigenvalue λ_n becomes zero. A typical eigenvector v_n has certain orthogonality properties:

$$v_m^T v_n = \delta_{mn} \tag{2.55}$$

and

$$\begin{aligned} v_m^T A v_n &= v_m^T \lambda_n v_n \\ &= \lambda_n v_m^T v_n \\ &= \lambda_n \delta_{mn} \end{aligned} \tag{2.56}$$

where the δ_{mn} denotes Kronecher's delta symbol.

Introducing the matrix V, the columns of which are the eigenvectors of A and the diagonal matrix Ω the element of which are the eigenvalues of A we can write

$$V^T A V = \Omega \qquad \text{or} \qquad A V = V \Omega \tag{2.57}$$

There are different numerical methods available to obtain the eigenvectors V and the associated eigenvalues Ω. In general, it is only necessary to find a certain number of smallest eigenvalues [59].

2.10.1 The Jacobi Method

This method is one of the oldest and most popular techniques for solving eigenvalue problems which was introduced in 1846. In this method the eigenvectors can be obtained from the following series of matrix multiplications.

$$V = T^{(0)} T^{(1)} \cdots T^{(k)} \cdots T^{(n-1)} T^{(n)} \tag{2.58}$$

where is assumed a unit matrix and $T^{(k)}$ is defined as orthogonal transformation matrix with four nonzero terms in different i and j rows and columns, [18] as indicated below:

$$\begin{bmatrix} - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - \\ - & - & T_{ii} & - & - & T_{ij} & - & - \\ - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - \\ - & - & T_{ji} & - & - & T_{jj} & - & - \\ - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - \end{bmatrix}$$

The four nonzero terms are the elements of an unknown rotation angle θ and defined as:

$$T_{ii} = T_{jj} = \cos\theta \qquad \text{and} \qquad T_{ji} = -T_{ij} = \sin\theta \tag{2.59}$$

Since the matrices $T^{(k)}$ are by definition normal matrices we have $\left(T^{(k)}\right)^T T^{(k)} = I$, which does not depend on θ. Here I stands for the identity matrix and the superscript T signifies transposition. The following matrix operation indicates the typical iteration, which enters our calculations:

$$A^{(k)} = T^{(k)T} A^{(k-1)} T^{(k)} \tag{2.60}$$

In order to force the terms (i, j) and (j, i) in the matrix $A^{(k)}$ becomes zero, the angle θ must be calculated as follow:

$$\tan 2\theta = \frac{2A_{ij}^{k-1}}{A_{ii}^{k-1} - A_{jj}^{k-1}} \tag{2.61}$$

This method can be applied to all off-diagonal terms sequentially. This method continues until all terms decays to smaller number in comparison with the absolute value of all matrix terms. In order to reduce an off-diagonal term to zero approximately 8N numerical operations are needed. The exact number of numerical operations is not predictable; however, experience has shown that the number of operations to achieve convergence is of the order of $10N^3$, [18].

2.10.2 Solution of General Eigenvalue Problems

Assume the following generalized eigenvalue problem:

$$AV = BV\Omega \tag{2.62}$$

Let A and B be both symmetric matrices. First we calculate the eigenvector of the matrix B. Now we can let V be a linear combination of the eigenvectors of matrix B. Therefore,

$$V = V_B\overline{V}. \tag{2.63}$$

By substituting (2.63) into (2.62) and multiplying both sides of the resulting equation by V_B^T, we obtain:

$$V_B^T A V_B \overline{V} = V_B^T B V_B \overline{V} \Omega \tag{2.64}$$

By normalizing $V_B^T B V_B = I$ (if there is no zero eigenvalue in matrix) equation (2.64) equals to the classical form:

$$\overline{A}\ \overline{V} = \overline{V} \Omega \tag{2.65}$$

Thus $\overline{A} = V_B^T A V_B$. Hence, Jacobi method can applied to both matrices. If matrix B is diagonal its eigenvector matrix (V_B) will be diagonal and the diagonal terms equal $1/\sqrt{B_{nn}}$ (assume $B_{nn} \neq 0$) [49], [50].

Chapter 3

Literature Review

3.1 Introduction

Possibly, the simplest answer to why we need to know about quantum mechanics is the fact that we are living in a quantum world [18]. Engineers would like to design electronic, optical and optoelectronic devices in atomic scale. In biology, they deal with cells and molecules which they wish to understand their motion and modify them in atomic scale. The same is true for chemistry in order to synthesize organic and inorganic compositions. Quantum mechanic provides the tool for those who are dealing with objects in atomic level [18].

Quantum mechanics is the basis of our present knowledge of physical phenomena in micro and nano scale. It provides a theoretical framework based on which it is feasible to correlate, demonstrate, and predict the behavior of large range of physical phenomena [19]. Quantum mechanics has a wide range of applications in different areas of science. For instance, in Engineering, it has great impact on various topics such as semiconductor transistors, lasers, and quantum optic [18].

With the advance of technology, it is predictable in the near future to have quantum devices such as single-electron memory cells. It is expected that new devices, with functionality based on principles of quantum mechanics, will be created [6], [18].

The small glimpse of our quantum world will reveal notable differences from our every-day life. Quiet often based on quantum view, the motion of objects does not follow our (classical) expectation [20], [41]. An interesting example is what happens when you throw a ball against a wall. We expect the ball to bounce back. Quantum mechanic has totally different view from what we expect. That is, under certain conditions, there is a possibility for the ball to pass through the wall. This is called tunnelling which is quantum mechanical effect and takes place due to the fact that on appropriate time and length scales particles are described as waves [18].

We will devote our attention in this thesis to quantum harmonic oscillator and its behavior when it is strongly perturbed. One may wonder why considerable effort has been dedicated to harmonic oscillator. The concept of quantum harmonic oscillator is far beyond a simple system [21]. It is so fundamental for quantum mechanics that in each and every quantum mechanical book one can find a chapter devoted to harmonic oscillator. In fact, the harmonic oscillator is one of the most important model systems in quantum mechanics. The most significant reason is the fact that any arbitrary potential can be approximated as a harmonic potential in the vicinity of its equilibrium point [4]. The indispensable reason for this applicability is that all systems in stable equilibrium perform harmonic motion around the equilibrium state for a small perturbations [21]. For instance, a radiation field behaves like a collection of harmonic oscillators [22].

Moreover, harmonic oscillator is one of few quantum mechanical systems for which we have an exact solution. The solution of harmonic oscillator has extensive applications in theoretical physics and chemistry. It is the foundation for describing complex modes of vibration in molecules and crystals, and the theory of electromagnetic field [3], [20].

A simple harmonic oscillator is characterized as a mass attached to a spring with its motion following a linear differential equation with constant coefficients [23]. This system has a restoring force which is proportional to the displacement from the equilibrium position (Hooke's Law).

In quantum mechanics the motion of a particle of mass m, in a potential $V(x)$ is illustrated by Schrödinger equation for the wave function $\psi(x)$ characterizing that particle. When the potential is $V(x) = kx^2$, this system represents a quantum harmonic oscillator [40].

3.2 Background Knowledge

Quantum Mechanics of a particle bound to the origin by an elastic potential kx^2 is of both practical and academic significance. In physical problems the motion of electromagnetic radiation, lattice vibration in solids, and molecular vibrations may be decompose into one dimensional harmonic oscillator [4]. Since any arbitrary potential can be approximated by a harmonic oscillator, it is important to investigate the characteristics of harmonic oscillator. This fundamental significance of harmonic oscillator for quantum mechanic has caused enormous attention and a large number of publications has been produced for this problem. When I searched the library of my university, I find

overwhelming number of books and journal publications related to quantum harmonic oscillator. This intense interest shows the continuing need for updated presentations of the material [24].

Because of the importance of harmonic oscillator, the classical as well as quantum harmonic oscillator has received renewed interest. Therefore, it can be seen that there are so many attempts for numerical and analytical approximation to the harmonic oscillator [25], [26], [27], [34], [35], [36]. Furthermore, for the eigenvalues of the bounded harmonic oscillator and hydrogen-type atoms several analytical approaches have been proposed [28], [38], [39].

The problem of a particle moving under the influence of a linear restoring force, $F(x) = -kx$ or a quadratic potential is one of those problems which have been studied at different levels of theoretical physics, from elementary classical mechanics to quantum field theory, [37]. As already mentioned, one of the most important features of such problems is the fact that it is exactly soluble. Therefore, it can be used as a closed-form, analytic example. Even if it had no practical usage for real-world physical systems, it would be of only academic interest [24]. In fact the solution of this problem has extensive application in theoretical physics and chemistry [3].

One of the important applications of this problem is its wide-ranging usefulness. By using standard differential equation approach the solution of harmonic oscillator in nonrelativististic quantum mechanics can be obtained.

The stationary state of harmonic oscillator is determined by two different methods. The

first one is the so-called Polynomial method in which the procedure is essentially the same as for the particle in a box. All possible mathematical solutions of a second-order of differential equation are first determined and then the physically permissible ones are selected. This method is called the classical method. A second approach, is called the algebraic method [3]. This method simply solve a first-order differential equation for the ground state. Then after, higher states are determined from the already known ground state by means of a ladder operator [3], [29]. The algebraic method plays an important role in modern quantum mechanics. In this thesis, we also utilize the algebraic method.

One dimensional systems are of interest for the fact that they illustrate some non-classical effects and even though we are living in a three dimensional world, many physical situations are effectively one dimensional [30]. Since harmonic oscillator is a fascinating system to study, perturbation of such system would be very interesting, indeed.

Undoubtedly the most widely used approximation method is perturbation theory. The notion of perturbation theory extends to quantum mechanics in cases where the observed system can be describe as an ‘‘unperturbed’’ Hamiltonian, for which eigenstates can be attained exactly [24]. In quantum mechanics, a perturbation usually refers to a slight variation in the potential function $V(x)$. Through the perturbation theory, the effect of perturbation on the states of the unperturbed potential can be obtained. These perturbed states can be acquired by having prior knowledge of the unperturbed ones.

It is a common practice to approach quantum mechanics through the study of a few exact soluble examples by using Schrödinger equation. The number of potential energy functions for which we have closed-form solutions is fairly small. Fortunately, most of the examples correspond relatively well to actual physical systems. For instance, one of the systems that has a closed-form solution which works very well with the actual system is the harmonic oscillator [24].

Nevertheless, it is good to pinpoint that other methods can be used to study the properties of a quantum system. Some of these methods are very different from the Schrödinger equation approach, and some others can be used as a numerical method for those problems for which analytical solutions are not available [24].

3.3 Perturbation Theory

As already mentioned, one of the methods of acquiring approximate solutions is the perturbation theory given by Schrödinger. This theory is an adjustment of a method developed by Rayleigh for the vibrating strings problem [5], [31]. For systems whose Hamiltonian is independent of time, time-independent Schrödinger equation is:

$$H\Psi_n = E_n\Psi_n \tag{3.1}$$

This theory is based on comparing the Hamiltonian H of the given system to an already solved system $H^{(0)}$, i.e.,

$$H^{(0)}\Psi_n^{(0)} = E_n^{(0)}\Psi_n^{(0)} \tag{3.2}$$

of which the set of eigenpairs (eigenvalues $E_n^{(0)}$ and the corresponding eigenfunctions $\Psi_n^{(0)}(x)$; $n \in N$) are known to us:

$$\left\{E_n^{(0)}, \Psi_n^{(0)} \middle| n \in N\right\}$$

Moreover, the functions $\Psi_n^{(0)}\,; n \in N$ are assumed to form a complete set of normalized and orthogonal functions. The difference $H - H^{(0)}$ is assumed to be small and expressed in the form

$$H = H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \cdots\,, \tag{3.3}$$

where λ is a parameter:

$$0 \leq \lambda \leq 1$$

Here, $\lambda = 0$ corresponds to zeroth-order system, equation (3.2), and $\lambda = 1$ corresponds to one degree perturbed. It is considered that eigenfunctions and eigenvalues can be expressed in the following form:

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \tag{3.4a}$$

$$\Psi_n = \Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \cdots \tag{3.4b}$$

in which $E_n^{(1)}, E_n^{(2)}, \cdots, \lambda\Psi_n^{(1)}, \lambda^2\Psi_n^{(2)}, \cdots$ are the first- and second- and higher perturbations due to $H^{(1)}, H^{(2)}, \cdots$, which need to be determined.

Substituting (3.3) and (3.4a) into (3.1) and equating the coefficients of various power of λ, we obtain

$$\lambda^0 : \quad H^{(0)}\Psi_n^{(0)} = E_n^{(0)}\Psi_n^{(0)} \tag{3.5a}$$

$$\lambda^1 : \quad H^{(0)}\Psi_n^{(1)} + H^{(1)}\Psi_n^{(0)} = E_n^{(0)}\Psi_n^{(1)} + E_n^{(1)}\Psi_n^{(0)} \tag{3.5b}$$

$$\lambda^2 : \quad H^{(0)}\Psi_n^{(2)} + H^{(1)}\Psi_n^{(1)} + H^{(2)}\Psi_n^{(0)} = E_n^{(0)}\Psi_n^{(2)} + E_n^{(1)}\Psi_n^{(1)} + E_n^{(2)}\Psi_n^{(0)} \tag{3.5c}$$

Then, we can proceed to calculate the functions $\Psi_n^{(1)}, \Psi_n^{(2)}, \cdots$ in succession [54], [55].

Assuming that the zeroth-order solution of the system is non-degenerate, that is, for different eigenstates, $\Psi_n^{(0)}$, we have different eigenvalues, $E_n^{(0)}$, we can write the following series expansion for $\Psi_n^{(1)}$:

$$\Psi_n^{(1)} = \sum_m a_{mn}\Psi_m^{(0)} \tag{3.6}$$

Substituting (3.6) into equation (3.5a), the eigenpairs (3.6) can be obtained [31]. Now, we are going to see how this method can be implemented. Our research focuses on one-

dimensional canonical and strongly perturbed quantum harmonic oscillator. We have utilized the solution of unperturbed harmonic oscillator as our gauging system in order to get an insight for the perturbed harmonic oscillator. In my view, it is very important to have a basic conceptual understanding of an alternative way of approaching linearly perturbed harmonic oscillator [4], and other monomially perturbed harmonic oscillator problems.

3.4 Standard Procedure for Tackling Linear Perturbation of Harmonic Oscillator

We will briefly describe the standard method and demonstrate how the technique is applied. The problem can be stated as follows:

The differential equation for linearly perturbed harmonic oscillator is set up. The original position variable x is replaced by a dimensionless variable ξ such that $\Psi = \Psi(\xi)$. Finding the eigenpairs of unperturbed harmonic oscillator leads to the construction of Hermite polynomials. A recurrence formula involving Hermite polynomials is then used to calculate the eigensolutions related to the linear perturbation of harmonic oscillator. Both sides of the recurrence equation are divided by 2, and an expression for $\xi\Psi_n$ is obtained in terms of Ψ_{n-1} and Ψ_{n+1}. Subsequently, this expression is implemented to calculate the influence of the perturbation caused by x. In the next section details of calculations are presented.

3.4.1 Numerical Calculations of Linearly Perturbed Harmonic Oscillator: Standard Way

For the sake of completeness and in order to avoid cross-referencing, the main result associated with ideal harmonic oscillator have been summarized.

Ideal (Unperturbed) Harmonic Oscillator

An unperturbed harmonic oscillator simply implies that figure (3.1) shows its original form. The problem is set up as the case of a particle constrained to move along the x-axis subject to an elastic potential proportional to a point located on that axis [32].

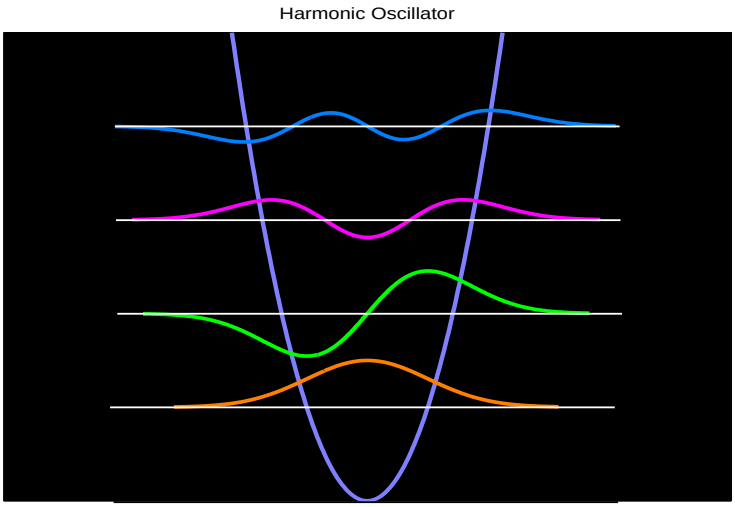

Figure 3.1: The Linearly Distributed Eigenvalues and the Corresponding Eigenfunctions of the Harmonic Oscillator

The harmonic oscillator can be solved by using Schrödinger equation

$$H\Psi = E\Psi, \tag{3.7}$$

where H is known as the Hamiltonian operator and corresponds to the total energy of the system [33]. Therefore, it corresponds to the sum of Kinetic and Potential Energy.

In the case of one-dimensional linear harmonic oscillator the hamiltonian operator is

$$H = \frac{1}{2m_0}p^2 + \frac{1}{2}m_0\omega^2 x^2 \tag{3.8}$$

To construct the quantum mechanical analogon x and p must be operators. Thereby, x is represented by x and p by $(\hbar/i)(d/dx)$.

Then Schrödinger equation for the harmonic oscillator is

$$\left(-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2} + \frac{1}{2}m_0\omega^2 x^2\right)\Psi = E\Psi \tag{3.9}$$

in which $\omega^2 = k/m_0$. The eigenfunctions of this Hamiltonian are real, non-degenerate, unique, and mutually orthogonal.

By changing variable x to be a dimensionless variable $\xi = \sqrt{\alpha}x$ where $\alpha = m_0\omega/\hbar$, equation (3.9) transforms to,

$$\frac{d^2}{d\xi^2}\Psi_n(\xi) + \left(\frac{\lambda_n}{\alpha} - \xi^2\right)\Psi_n(\xi) = 0 \tag{3.10}$$

where $\lambda_n = 2m_0E_n/\hbar^2$. Those solutions that satisfy $\Psi_n(\pm\infty) = 0$ are acceptable.

Next, a solution of the form is assumed

$$\Psi = G(\xi)H(\xi) \tag{3.11}$$

where $G(\xi)$ is a function describing general behavior of Ψ for large $|\xi|$ and $H(\xi)$ is an infinite series.

These considerations lead to the result

$$\Psi_n(\xi) = N_n e^{-\xi^2/2} H_n(\xi), \tag{3.12}$$

where N_n is the normalization constant,

$$N_n = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(\frac{1}{2^n n!}\right)^{1/2} \tag{3.13}$$

Linearly Anharmonic Oscillator

Sketch of the idea:

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\widetilde{\psi} + \frac{1}{2}kx^2\widetilde{\psi} + \beta x\widetilde{\psi} = E\widetilde{\psi} \tag{3.14}$$

going through our procedure:

We need to calculated interaction matrices of the form

$$\begin{aligned}\langle\psi_m\big|x\big|\psi_n\rangle &= \int dx N_m e^{-x^2/2}\, H_m(x)\, x\, N_n e^{-x^2/2}\, H_n(x) \\ &= N_m\, N_n \int dx\, x\, H_m(x)\, H_n(x) e^{-x^2} \end{aligned} \tag{3.15}$$

Then, $\xi = \sqrt{\alpha}x$ is introduced. Using the recurrence property of Hermite polynomials, i.e.

$$H_{n+1}(\xi) - 2\xi H_n(\xi) + 2nH_{n-1}(\xi) = 0, \tag{3.16}$$

Multiplying both side of the above equation by $e^{-\xi^2}$ and dividing to 2, the following relation can be obtained

$$\xi H_n(\xi) = nH_{n-1}(\xi) + \frac{1}{2}H_{n+1}(\xi) \tag{3.17}$$

which can be implemented in the following equation which are the matrix elements of $\hat{x}$:

$$\begin{aligned}\langle\psi_m\big|\xi\big|\psi_n\rangle &= \frac{1}{\alpha}\, N_m\, N_n \int d\xi\, H_m(\xi)\, \left[nH_{n-1}(\xi) + \frac{1}{2}H_{n+1}(\xi)\right] e^{-x^2} \\ &= \frac{1}{\alpha}\, N_m\, N_n \left\{\frac{1}{2}\int d\xi\, H_m(\xi)\, H_{n+1}(\xi)\, e^{-x^2} + n\int d\xi\, H_m(\xi)\, H_{n-1}(\xi)\, e^{-x^2}\right\} \\ &= \frac{1}{\alpha}\, N_m\, N_n \left\{\frac{1}{2}\delta_{m,n+1} + n\delta_{m,n-1}\right\} \end{aligned} \tag{3.18}$$

Substituting equation (3.17) into (3.18), the matrix elements result in

$$\langle\psi_m|\hat{x}|\psi_n\rangle = \frac{N_n}{N_{n-1}}\frac{n}{\sqrt{\alpha}}\delta_{m,n-1} + \frac{N_n}{N_{n+1}}\frac{n}{\sqrt{\alpha}}\delta_{m,n+1}. \tag{3.19}$$

The only nonvanishing matrix elements are

$$\langle\psi_{n-1}|\hat{x}|\psi_n\rangle = \sqrt{\frac{n\hbar}{2m_0\omega}} \tag{3.20a}$$

$$\langle\psi_{n+1}|\hat{x}|\psi_n\rangle = \sqrt{\frac{(n+1)\hbar}{2m_0\omega}}. \tag{3.20b}$$

Therefore, it can be shown in matrix form as follow:

$$\hat{x} \longrightarrow \left(\frac{\hbar}{2m_0\omega}\right)^{1/2} \begin{bmatrix} 0 & \sqrt{1} & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{3.21}$$

As will be shown in Chapter 4 our formulation is valid for arbitrary monomial perturbation βx^r of order r, by construction includes the case $r = 1$ and results in the ‘‘system’’ matrix given in (3.21).

The above calculation was for linear perturbation of harmonic oscillator [4] but our method of computation extend the perturbation for any arbitrary perturbation monomial with an arbitrary coefficient.

In the following, I will provide a brief outline of the topics which will be covered in Chapters 4 -7.

In Chapter 4 of this thesis, we demonstrate our method of solving perturbation on harmonic oscillator. The uniqueness of our method is due to the flexibility that gives us to calculate arbitrary perturbation monomials with arbitrary coefficients. At the beginning section of the following chapter, we demonstrate our method of obtaining the solutions of the unperturbed harmonic. The following section is devoted to determining the solution of the anharmonic oscillator. Finally, last section of Chapter 4 details the calculation of the involved integrals which we introduces.

In Chapter 5, the numerical results obtained are discussed thoroughly. We divide these numerical results in two main categories based on the power of the perturbation monomial to be odd or even.

In Chapter 6, we point to some new problems which can be solved based on our methodology.

Finally, in Chapter 7, we summarize the work emphasizing the achievements in this research.

Chapter 4

Anharmonic Oscillator

4.1 Introduction

In this chapter, we focus on solving the following monomially perturbed harmonic oscillator problem:

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\widetilde{\varphi}(x)+\left(\frac{1}{2}kx^2+\widetilde{\beta}x^r\right)\widetilde{\varphi}(x)=\widetilde{E}\widetilde{\varphi}(x) \tag{4.1}$$

In this equation the term $\widetilde{\beta}x^r$ is the perturbation with arbitrary $\widetilde{\beta}$ and $r \geq 1$. Our method consists of, in the first step, the determination of the eigenvalues and the corresponding eigenfunctions of the unperturbed harmonic oscillator. To this end we use the standard techniques, which result in closed-form for the eigenfunctions, eigenstates and linearly distributed eigenvalues. The complete set of eigensolutions of the harmonic oscillator can be calculated in analytical form using Hermite polynomials [1]. Having determined the solutions of this ‘‘auxiliary problem’’, we then proceed to solve our anharmonic oscillator. Therefore, our method is based upon using the eigensolutions

of the unperturbed harmonic oscillator as auxiliary (gauging) functions. The obtained eigenfunctions of the unperturbed harmonic oscillator can be used as a complete set of functions for analyzing related boundary value problems, in particular the family of problems given in (4.1). Thereby, the key idea is the construction of an appropriately devised auxiliary problem the eigenpairs, which in the present case is the ideal harmonic oscillator. As it will become apparent the applicability range of the concept presented here is quite large. More challenging cases have been announced at the end of the manuscript.

In summary, in this chapter we will describe our methodology for solving perturbed harmonic oscillator. In the first two sections calculation of eigenfunctions $\psi(\xi)$ and corresponding eigenvalue $\widehat{E}$ for unperturbed harmonic oscillator will be discussed. Thereby, the replacement of the coordinate x by an appropriately introduced nondimensional variable ξ plays a significant role, as is known from standard text books. Thereby, the determination of $\psi_m(\xi)$ and corresponding $\widehat{E}_m$ will be facilitated by the help of annihilation and creation operators. The annihilation and creation operators are discussed in detail in the same section. In the following section, our objective will be the determination of the solution of perturbed harmonic oscillator, i.e. the eigenfunction $\widetilde{\psi}_m(\xi)$ and the corresponding eigenvalues $\widehat{\widetilde{E}}_m$. For the calculation of perturbed eigenfunction and corresponding eigenvalues, we have developed a very novel recursion formula for the closed-form evaluation of the involved definite integrals. These integral calculations are discussed in the final section of this chapter.

4.2 Normalized Eigenfunctions $\psi_m(\xi)$ and the Corresponding Normalized Eigenvalues $\widehat{\boldsymbol{E}}_m$ of an Harmonic Oscillator

In the following subsections, we will describe the steps for the computation of the eigenvalues and corresponding eigenfunctions of the unperturbed harmonic oscillator,these ''auxiliary'' results are then used for the determination of the eigenstates of the perturbed harmonic oscillator.

4.2.1 Eigenvalues $\widehat{\boldsymbol{E}}_m$

Consider the harmonic motion of a particle with mass m in the parabolic potential energy function $V(x)$ given by

$$V(x) = \frac{1}{2}kx^2. \tag{4.2}$$

Assuming the validity of the Hook's Law for the linearized spring in our problem, k represents the spring constant. Newton's equation of motion dictates that the equation for a point with mass m_0 attached to spring with the spring constant k is:

$$m_0\ddot{x} = -kx \tag{4.3}$$

Assuming a harmonic time-dependence according to $x = e^{-j\omega t}$ and substituting into equation (4.3) we obtain

$$m_0\omega^2 = k, \tag{4.4}$$

or, alternatively,

$$\omega = \sqrt{\frac{k}{m_0}}. \tag{4.5}$$

Here, ω stands for the angular frequency of oscillations.

The Hamiltonian function of our system is (the total energy)

$$H = \frac{p^2}{2m_0} + V(x) \tag{4.6}$$

Using the particle/wave duality principle

$$p = \hbar k \tag{4.7a}$$

$$E = \hbar\omega \tag{4.7b}$$

and using the hypothesis that energy observable in classical physics has a corresponding operator in quantum mechanics according to

$$x \iff x \tag{4.8a}$$

$$V(x) \iff V(x) \tag{4.8b}$$

$$p \iff \frac{\hbar}{j}\frac{\partial}{\partial x} \tag{4.8c}$$

$$E \iff -\frac{\hbar}{j}\frac{\partial}{\partial t} \tag{4.8d}$$

and using the time-harmonic dependence($e^{j\omega t}$), we arrive at the time-dependent Schrödinger equation:

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\varphi(x) + V(x)\varphi(x) = E\,\varphi(x) \tag{4.9}$$

Here, $\hbar$ denotes the reduced Planck's constant $\hbar = h/(2\pi)$ with h standing for the Planck's constant h. The potential function $V(x)$, as expressed in equation (4.2) is $1/2kx^2$ in the current problem. We obtain:

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\varphi(x) + \frac{1}{2}m_0\,\omega^2\,x^2\varphi(x) = E\,\varphi(x) \tag{4.10}$$

As will be seen shortly the following variable transformation allows the simplification of calculations considerably:

$$x = \frac{1}{\sqrt{\alpha}}\,\xi \tag{4.11}$$

Introducing the function $\psi(\xi)$

$$\varphi(x) = \psi(\xi) \tag{4.12}$$

We can write,

$$\begin{aligned} \frac{d}{dx}\varphi(x) &= \frac{d}{dx}\psi(\xi) && (4.13a) \\ &= \frac{d\xi}{dx}\frac{d}{d\xi}\psi(\xi) && (4.13b) \end{aligned}$$

taking into account (4.11) we arrive at:

$$\frac{d}{dx} = \sqrt{\alpha}\frac{d}{d\xi} \tag{4.14}$$

proceeding similarly we obtain

$$\frac{d^2}{dx^2} = \alpha\,\frac{d^2}{d\xi^2}. \tag{4.15}$$

Using the above results and factorizing out the term $m_0\omega^2/\alpha$ equation (4.10) leads to

$$\frac{m_0\omega^2}{\alpha}\left[-\frac{\alpha}{m_0\omega^2}\frac{\hbar^2}{2m_0}\alpha\frac{d^2}{d\xi^2}\psi(\xi) + \frac{1}{2}\xi^2\psi(\xi)\right] = E\,\psi(\xi). \tag{4.16}$$

Setting the coefficient of differential term equal to unity, we obtain the following value for α:

$$\frac{\hbar^2\alpha^4}{{m_0}^2\omega^2} = 1 \quad \Longrightarrow \quad \alpha = \frac{m_0\omega}{\hbar} \tag{4.17}$$

The multiplicative factor in front of the square bracket in (4.16) has consequently the value

$$\frac{m_0\omega^2}{\alpha} = m_0{\omega}^2\frac{\hbar}{m_0\omega} \tag{4.18a}$$

$$= \hbar\omega. \tag{4.18b}$$

These considerations lead to the result:

$$\hbar\omega\left[-\frac{1}{2}\,\frac{d^2}{d\xi^2}\,\psi(\xi) + \frac{1}{2}\xi^2\,\psi(\xi)\right] = E\,\psi(\xi) \tag{4.19}$$

Dividing both sides of this equation by $\hbar\omega$ and introducing the dimensionless variable $\widehat{E} = E/\hbar\omega$, we obtain

$$\frac{1}{2}\left[-\frac{d^2}{d\xi^2}\psi(\xi) + \xi^2\,\psi(\xi)\right] = \widehat{E}\psi(\xi). \tag{4.20}$$

In the following we will aim at finding othomalised eigenfunctions of the equation (4.20) in the sense:

$$\Big\langle\, \varphi_m(x) \,\Big|\, \varphi_n(x) \Big\rangle = \delta_{mn}, \tag{4.21}$$

where δ_{mn} denotes Kronecher's delta symbol.

The term in the square bracket at the left-hand side of equation (4.20) can be written as

$$-\frac{d^2}{d\xi^2} + \xi^2 = \left(-\frac{d}{d\xi} + \xi\right)\left(\frac{d}{d\xi} + \xi\right) + I \tag{4.22}$$

where I denotes the identity operator: $If(\xi) = f(\xi)$.

By normalizing the operators at the right-hand side on equation (4.22), we can obtain normalized annihilation and creation operators a and $a^\dagger$ which are differential operators and are defined as,

$$a = \frac{1}{\sqrt{2}}\left(\frac{d}{d\xi} + \xi\right) \tag{4.23}$$

and

$$a^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{d}{d\xi} + \xi\right) \tag{4.24}$$

The reason why these operators are referred to as the annihilation and creation operators has been discussed in detail in Chapter 2 of this thesis, where also their importance are also addressed.

Apply the composed operator $aa^\dagger$ to the wave function $\psi(\xi)$ we obtain:

$$a\,a^{\dagger}\,\psi(\xi) = \frac{1}{2}\left[-\frac{d^2}{d\xi^2}\,\psi(\xi) + \xi^2\,\psi(\xi) - \psi(\xi)\right] \tag{4.25}$$

Alternatively, the application of $a^{\dagger}\,a$ to $\psi(\xi)$ results in:

$$a^{\dagger}\,a\,\psi(\xi) = \frac{1}{2}\left[-\frac{d^2}{d\xi^2}\,\psi(\xi) + \xi^2\,\psi(\xi) + \psi(\xi)\right] \tag{4.26}$$

- A comparison between the last two equations reveals the following equation:

$$a\,a^{\dagger}\,\psi(\xi) - a^{\dagger}\,a\,\psi(\xi) = \psi(\xi) \tag{4.27}$$

  Since this identity is valid for any permissible not identically vanishing wave function $\psi(\xi)$ the following identity for the a and $a^{\dagger}$ can be deduced:

$$a\,a^{\dagger}\, - a^{\dagger}\,a\, = I \tag{4.28}$$

- Schrödinger equation can be expressed as,

$$a^{\dagger}\,a\,\psi(\xi) = \left(\widehat{E} - \frac{1}{2}\right)\psi(\xi) \tag{4.29}$$

  since,

$$-\frac{1}{2}\,\frac{d^2}{d\xi^2} + \frac{1}{2}\,\xi^2\, = \left(a^{\dagger}\,a\, + \frac{1}{2}\right) \tag{4.30}$$

- In particular the solution of the differential equation

$$a\,\psi(\xi) = 0 \tag{4.31a}$$

$$\left(\frac{d}{d\xi} + \xi\right)\psi(\xi) = 0 \tag{4.31b}$$

is denoted $\psi_0(\xi)$ and is given

$$\psi_0(\xi) = A\,e^{-\xi^2/2}. \tag{4.32}$$

Which is seen immediately by substituting $\psi_0(\xi)$ into equation (4.31b). A can be determined by the normalization condition, equation (4.21), the constant resulting in

$$A = 1/\sqrt[4]{\pi}.$$

It is easily seen that $\widehat{E}_0 = 1/2$ is corresponding eigenvalue to the eigenfunction $\psi_0(\xi)$,

$$\left(a^\dagger a + \frac{1}{2}\right)\psi(\xi) = \widehat{E}\psi(\xi) \tag{4.33a}$$

$$\left(a^\dagger a\right)\psi(\xi) = \left(\widehat{E} - \frac{1}{2}\right)\psi(\xi) \tag{4.33b}$$

which can be written in the following correspondence form:

$$\psi_0(\xi)\left(= \frac{1}{\sqrt[4]{\pi}}\,e^{-\xi^2/2}\right) \iff \frac{1}{2} \tag{4.34}$$

- It is immediate to see that the function $a^\dagger\psi_0$ is a solution of Schrödinger equation belonging to the eigenvalue $\widehat{E} = 3/2$.

  To demonstrate this result and its generalization, we proceed as follows

$$a^\dagger\, a\, \psi(\xi) = \left(\widehat{E} - 1/2\right) \psi(\xi) \tag{4.35}$$

  Substitute for $\psi(\xi)$ the solution $\psi_n(\xi)$ with $\widehat{E}_n$ as its eigenvalue

$$a^\dagger\, a\, \psi_n(\xi) = \left(\widehat{E}_n - 1/2\right) \psi_n(\xi) \tag{4.36}$$

  with

$$\psi_n(\xi) \Longleftrightarrow \widehat{E}_n - 1/2 \tag{4.37}$$

  Multiplying both sides of the equation (4.36) by $a^\dagger$

$$a^\dagger a^\dagger\, a\, \psi_n(\xi) = \left(\widehat{E}_n - 1/2\right) a^\dagger\psi_n(\xi) \tag{4.38}$$

  Using equation (4.28) in (4.38)

$$a^\dagger \left(a\, a^\dagger - I\right)\, \psi_n(\xi) = \left(\widehat{E}_n - 1/2\right) a^\dagger\psi_n(\xi) \tag{4.39}$$

  and bringing the term $a^\dagger\psi_n$ to the right-hand side we obtain:

$$a^\dagger\, a\, a^\dagger\, \psi_n(\xi) = \left(\widehat{E}_n - \frac{1}{2} + 1\right) a^\dagger\psi_n(\xi) \tag{4.40}$$

which implies

$$a^\dagger \psi_n(\xi) \Longleftrightarrow \widehat{E}_n - \frac{1}{2} + 1 \tag{4.41}$$

meaning that $a^\dagger \psi_n$ is an eigenfunction of the Schrödinger equation with the corresponding eigenvalue $\widehat{E}_n - \frac{1}{2} + 1$ which is higher than the eigenvalue of ψ_n $(\widehat{E}_n - 1/2)$ by one. Therefore,

$$a^\dagger \psi_n(\xi) = \psi_{n+1} \tag{4.42}$$

Analogously, it can be shown that

$$a^\dagger \psi_n(\xi) = \psi_{n+1}(\xi) \Longleftrightarrow \widehat{E}_n - \frac{1}{2} + 1 \tag{4.43}$$

Therefore,

$$\psi_m(\xi) \iff (m + 1/2) \tag{4.44}$$

In this section, we have obtained an expression for E_m which is eigenvalue of the unperturbed harmonic oscillator.

4.2.2 Eigenfunction $\psi_m(\xi)$

The ‘‘ground state’’ for the harmonic oscillator has the form

$$\psi_0(\xi) = A_0 e^{-\xi^2/2} \tag{4.45}$$

where $A_0 = 1/\sqrt[4]{\pi}$.

Applying the creation operator on $\psi_0(\xi)$ will obtain the first excited state. Therefore, n-times application of creation operator on $\psi_0(\xi)$ will produce n^{th} excited state. To elucidate these ideas consider the following calculations:

Application of a on the ground state $\psi_0(\xi)$

$$\psi_0(\xi) = A_0 e^{-\xi^2/2} \tag{4.46}$$

With A_0 being a constant.

Ground state can be shown,

$$\begin{aligned} a\psi_0(\xi) &= \left(\frac{d}{d\xi} + \xi\right) A_0 e^{-\xi^2/2} \\ &= -A_0 \xi e^{-\xi^2/2} + \xi A_0 e^{-\xi^2/2} && (4.47a) \\ &= 0 && (4.47b) \end{aligned}$$

For the first excited state, we have

$$\begin{aligned} a^\dagger \psi_0(\xi) &= \left(-\frac{d}{d\xi} + \xi\right) A_0 e^{-\xi^2/2} \\ &= -\frac{d}{d\xi} A_0 e^{-\xi^2/2} + \xi A_0 e^{-\xi^2/2} \qquad (4.48a) \\ &= \psi_1(\xi) \qquad (4.48b) \end{aligned}$$

For the second excited state,

$$\begin{aligned} a^\dagger \psi_1(\xi) &= \left(-\frac{d}{d\xi} + \xi\right) 2A_0 \xi e^{-\xi^2/2} \\ &= -\frac{d}{d\xi} 2A_0 \xi e^{-\xi^2/2} + 2A_0 \xi^2 e^{-\xi^2/2} \\ &= (-2 + 4\xi^2)\psi_0(\xi) \qquad (4.49a) \\ &= \psi_2(\xi) \qquad (4.49b) \end{aligned}$$

By applying the creation operator $a = (-d/d\xi + \xi)$ m-times onto $\psi_0(\xi)$, we obtain the expression for m^{th} ''excited state'' $\psi_m(\xi)$ along with its corresponding eigenvalue $\widehat{E}_m$. Therefore, for the normalized eigenfunction $\psi_m(\xi)$ we obtain:

$$\psi_m(\xi) = \frac{1}{\sqrt{\sqrt{\pi} m! 2^m}} H_m(\xi) e^{-\xi^2/2} \qquad (4.50)$$

where $H_m(\xi)$ $(m \in N)$ stands for the normalized Hermite polynomials which are discussed in detail in Chapter 2, Section 2.5.

By utilizing the solutions of harmonic oscillator as our chosen auxiliary boundary value problem, we next focus on the perturbed harmonic oscillator problem.

4.3 Schrödinger Equation for Monomially Perturbed Harmonic Oscillators

The hamiltonian for 1D harmonic oscillator is

$$H = \frac{p^2}{2m_0} + \frac{m_0\omega^2 x^2}{2} \tag{4.51}$$

Then, the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\varphi(x) + \frac{1}{2}kx^2\varphi(x) = \widehat{E}\varphi(x) \tag{4.52}$$

We introduce a new dimensionless variable ξ by changing the scale of $x = \sqrt{\alpha}\xi$ where α will be chosen such that we obtain a simpler coefficients in that differential equation (4.52). Consequently, we changed $\varphi(x)$ to $\psi(\xi)$. The solution of equation (4.52) with the new variable ξ i.e. eigenfunction $\psi_m(\xi)$ and the corresponding eigenvalue $\widehat{E}_m$) were discussed in detail in the Section (4.2).

As we found out, the time-independent Schrödinger equation had the form

$$-\frac{1}{2}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}\psi(x) = \widehat{E}\psi(x) \tag{4.53}$$

let our perturbed harmonic oscillator has the form,

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\widetilde{\varphi}(x)+\frac{1}{2}m_0\omega^2x^2\widetilde{\varphi}(x)+\widetilde{\beta}x^r\widetilde{\varphi}(x)=\widetilde{E}\,\widetilde{\varphi}(x) \tag{4.54}$$

where the perturbation coefficient $\widetilde{\beta}$ stands for

$$\widetilde{\beta}=\hbar\omega\left(\frac{m_0\omega}{\hbar}\right)^{r/2}\beta \tag{4.55}$$

By replacing the following substitution into equation (4.54),

$$\widetilde{\varphi}(x)=\widetilde{\psi}(\xi),\qquad x=\frac{1}{\sqrt{\alpha}}\xi\qquad\text{and}\qquad\frac{d}{dx}=\sqrt{\alpha}\frac{d}{d\xi} \tag{4.56}$$

equation (4.54) transforms into,

$$-\frac{\hbar^2}{2m_0}\alpha\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)+\frac{1}{2}m_0\omega^2\frac{1}{\alpha}\xi^2\widetilde{\psi}(\xi)+\hbar\omega\sqrt{\left(\frac{m_0\omega}{\hbar}\right)^r}\beta\frac{1}{\alpha^{r/2}}\xi^r\widetilde{\psi}(\xi)=\widetilde{E}\,\widetilde{\psi}(\xi) \tag{4.57}$$

Factorizing out the term $m_0\omega^2/\alpha$ in equation (4.57), we have

$$\frac{m_0\omega^2}{\alpha}\left[-\frac{\alpha}{m_0\omega^2}\frac{\hbar^2}{2m_0}\alpha\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)+\frac{1}{2}\xi^2\widetilde{\psi}(\xi)+\frac{\alpha}{m_0\omega^2}\hbar\omega\sqrt{\left(\frac{m_0\omega}{\hbar}\right)^r}\beta\frac{1}{\alpha^{r/2}}\xi^r\widetilde{\psi}(\xi)\right]=\widetilde{E}\,\widetilde{\psi}(\xi). \tag{4.58}$$

Again, if we set the coefficient of the first term in the square bracket in (4.58) to 1, we obtain

$$\alpha = \frac{m_0\omega}{\hbar}. \tag{4.59}$$

By substituting α into equation (4.58), we have

$$\hbar\omega\left[-\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \frac{1}{2}\xi^2\widetilde{\psi}(\xi) + \beta\xi^r\widetilde{\psi}(\xi)\right] = \widetilde{E}\,\widetilde{\psi}(\xi), \tag{4.60}$$

which is equal to,

$$-\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \frac{1}{2}\xi^2\widetilde{\psi}(\xi) + \beta\xi^r\widetilde{\psi}(\xi) = \widehat{\widetilde{E}}\,\widetilde{\psi}(\xi) \tag{4.61}$$

Therefore, this equation is the scaled $\left(x = \sqrt{\hbar/m_0\omega}\xi\right)$ version of

$$-\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2}\widetilde{\varphi}(x) + \frac{1}{2}m_0\omega^2x^2\widetilde{\varphi}(x) + \hbar\omega\sqrt{\left(\frac{m_0\omega}{\hbar}\right)^r}\beta x^r\widetilde{\varphi}(x) = \widetilde{E}\,\widetilde{\varphi}(x) \tag{4.62}$$

4.3.1 Proposed Methodology

Auxiliary Problem: The differential equation for the harmonic oscillator obtained in equation (4.20) is:

$$-\frac{1}{2}\frac{d^2}{d\xi^2}\psi(\xi) + \frac{1}{2}\xi^2\psi(\xi) = \widehat{E}\psi(\xi) \tag{4.63}$$

We shall consider the eigenpairs $\{\psi_m, \widehat{E}_m\}$ of this problem as our gauging system. This

is the reason why we will refer to (4.63) as our auxiliary problem.

Actual problem: Our actual (original) problem is a perturbation of the harmonic oscillator by an additive monomial potential function. Here, we consider general monomials of the form $\beta\xi^r$ with r being an integer and β a positive constant specifying the magnitude of the perturbation. The differential equation characterizing our actual problem has therefore the form:

$$-\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)+\frac{1}{2}\xi^2\widetilde{\psi}(\xi)+\beta\xi^r\widetilde{\psi}(\xi)=\widehat{\widetilde{E}}\widetilde{\psi}(\xi) \tag{4.64}$$

Our objective is the solution of (4.64) and thus the determination of eigenfunctions $\widetilde{\psi}_m(\xi)$ and the corresponding eigenvalues $\widehat{\widetilde{E}}_m$. To this end we proceed as follows:

Multiply the auxiliary system by $\widetilde{\psi}(\xi)$ and the actual problem by $\psi(\xi)$ and subtract the resulting ''actions'' obtaining:

$$-\begin{cases} -\widetilde{\psi}(\xi)\frac{d^2}{d\xi^2}\psi(\xi)+\frac{1}{2}\widetilde{\psi}(\xi)\xi^2\psi(\xi)=\widehat{E}\widetilde{\psi}(\xi)\psi(\xi) \\ \\ -\psi(\xi)\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)+\frac{1}{2}\psi(\xi)\xi^2\widetilde{\psi}(\xi)+\beta\psi(\xi)\xi^r\widetilde{\psi}(\xi)=\widehat{\widetilde{E}}\psi(\xi)\widetilde{\psi}(\xi) \end{cases}$$

We obtain:

$$-\widetilde{\psi}(\xi)\frac{d^2}{d\xi^2}\psi(\xi)-\psi(\xi)\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)-\beta\xi^r\psi(\xi)\widetilde{\psi}(\xi)=\left(\widehat{E}-\widehat{\widetilde{E}}\right)\psi(\xi)\widetilde{\psi}(\xi) \tag{4.66}$$

By integrating both sides of this equation from $-\infty$ to $+\infty$, we have

$$
\begin{aligned}
- & \int_{-\infty}^{+\infty} d\xi \left(\widetilde{\psi}(\xi) \frac{d^2}{d\xi^2} \psi(\xi) - \psi(\xi) \frac{d^2}{d\xi^2} \widetilde{\psi}(\xi) \right) - \int_{-\infty}^{+\infty} d\xi \beta \xi^r \psi(\xi) \widetilde{\psi}(\xi) \\
= & \int_{-\infty}^{+\infty} d\xi \left(\widehat{E} - \widehat{\widetilde{E}} \right) \psi(\xi) \widetilde{\psi}(\xi)
\end{aligned} \tag{4.67}
$$

It is instructive to introduce I and J as follows:

$$
I = \int_{-\infty}^{+\infty} d\xi \widetilde{\psi}(\xi) \frac{d^2}{d\xi^2} \psi(\xi), \tag{4.68}
$$

and

$$
J = \int_{-\infty}^{+\infty} d\xi \psi(\xi) \frac{d^2}{d\xi^2} \widetilde{\psi}(\xi), \tag{4.69}
$$

First we calculate I as follow:

$$
I = \int_{-\infty}^{+\infty} d\xi \widetilde{\psi}(\xi) \frac{d^2}{d\xi^2} \psi(\xi) \tag{4.70}
$$

Using the identity

$$
d(uv) = udv + vdu \tag{4.71}
$$

we can write

$$\int_a^b d(uv) = \int_a^b udv + \int_a^b vdu \qquad \Longrightarrow \qquad uv\Big|_a^b = \int_a^b udv + \int_a^b vdu \tag{4.72}$$

for the partial integration.

Therefore,

$$\begin{aligned} I &= \int_{-\infty}^{+\infty} d\xi \underbrace{\widetilde{\psi}(\xi)}_{u} \underbrace{\frac{d}{d\xi}\frac{d}{d\xi}\psi(\xi)}_{v'} \\ &= \widetilde{\psi}(\xi)\frac{d}{d\xi}\psi(\xi)\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} d\xi \left\{\frac{d}{d\xi}\widetilde{\psi}(\xi)\right\}\left\{\frac{d}{d\xi}\psi(\xi)\right\} \end{aligned} \tag{4.73}$$

Since $\widetilde{\psi}(+\infty) = \widetilde{\psi}(-\infty) = 0$:

$$I = -\int_{-\infty}^{+\infty} d\xi \left\{\frac{d}{d\xi}\widetilde{\psi}(\xi)\right\}\left\{\frac{d}{d\xi}\psi(\xi)\right\} \tag{4.74}$$

Applying the same procedure to J, we arrive at

$$\begin{aligned} J &= \int_{-\infty}^{+\infty} d\xi \underbrace{\psi(\xi)}_{u} \underbrace{\frac{d}{d\xi}\frac{d}{d\xi}\widetilde{\psi}(\xi)}_{v'} \\ &= \psi(\xi)\frac{d}{d\xi}\widetilde{\psi}(\xi)\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} d\xi \left\{\frac{d}{d\xi}\psi(\xi)\right\}\left\{\frac{d}{d\xi}\widetilde{\psi}(\xi)\right\} \end{aligned} \tag{4.75}$$

Again imposing the conditions $\psi(+\infty) = \psi(-\infty) = 0$ result in

$$J = -\int_{-\infty}^{+\infty} d\xi \left\{ \frac{d}{d\xi}\psi(\xi) \right\} \left\{ \frac{d}{d\xi}\widetilde{\psi}(\xi) \right\} \tag{4.76}$$

Consequently, $I{=}J$ and thus

$$-\int_{-\infty}^{+\infty} d\xi \left(\widetilde{\psi}(\xi)\frac{d^2}{d\xi^2}\psi(\xi) - \psi(\xi)\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) \right) = 0. \tag{4.77}$$

With this result equation (4.67) is:

$$-\int_{-\infty}^{+\infty} d\xi\beta\xi^r\psi(\xi)\widetilde{\psi}(\xi) = \int_{-\infty}^{+\infty} d\xi \left(\widehat{E} - \widehat{\widetilde{E}} \right) \psi(\xi)\widetilde{\psi}(\xi) \tag{4.78}$$

or,

$$\beta\int_{-\infty}^{+\infty} d\xi\xi^r\psi(\xi)\widetilde{\psi}(\xi) = \left(\widehat{\widetilde{E}} - \widehat{E} \right) \int_{-\infty}^{+\infty} d\xi\psi(\xi)\widetilde{\psi}(\xi) \tag{4.79}$$

In particular choosing $\psi_m(\xi)$ $(m \in N)$ for $\psi(\xi)$ we have

$$\beta\int_{-\infty}^{+\infty} d\xi\xi^r\psi_m(\xi)\widetilde{\psi}(\xi) = \left(\widehat{\widetilde{E}} - \widehat{E}_m \right) \int_{-\infty}^{+\infty} d\xi\psi(\xi)\widetilde{\psi}(\xi) \tag{4.80}$$

Using the completeness property of the set of functions $\{\psi_n(\xi)\}$, we can write the following series expansion for $\widetilde{\psi}(\xi)$ with *a priori* expansion coefficients α_n

$$\widetilde{\psi}(\xi) = \sum_{n=0}^{\infty} \alpha_n\psi_n(\xi) \tag{4.81}$$

Substituting (4.81) into (4.80) results in

$$\beta \int_{-\infty}^{+\infty} d\xi \xi^r \psi_m(\xi) \sum_{n=0}^{\infty} \alpha_n \psi_n(\xi) = \left(\widehat{\widehat{E}} - \widehat{E}_m \right) \int_{-\infty}^{+\infty} d\xi \psi_m(\xi) \sum_{n=0}^{\infty} \alpha_n \psi_n(\xi) \tag{4.82}$$

We know that $\widehat{E} = E/\hbar\omega$ and $E_m = (m + 1/2)\hbar\omega$; therefore, $\widehat{E}_m = (m + 1/2)$, which result in

$$\beta \sum_{n=0}^{\infty} \alpha_n \langle \psi_m(\xi) | \xi^r | \psi_n(\xi) \rangle = \left[\widehat{\widehat{E}} - (m + 1/2) \right] \sum_{n=0}^{\infty} \alpha_n \langle \psi_m(\xi) | \psi_n(\xi) \rangle \tag{4.83}$$

right hand side of equation (4.83) can be named in the following form,

For the ‘‘interaction’’ matrix element (the term in the angled brackets) we write

$$A^r_{mn} = \langle \psi_m(\xi) | \xi^r | \psi_n(\xi) \rangle. \tag{4.84}$$

Writing the explicit expression for $\psi_m(\xi)$ and $\psi_n(\xi)$ we obtain:

$$\begin{aligned} &\beta \sum_{n=0}^{\infty} \alpha_n \int_{-\infty}^{+\infty} d\xi \frac{1}{\sqrt{\sqrt{\pi} m! 2^m}} H_m(\xi) e^{-\xi^2/2} \xi^r \frac{1}{\sqrt{\sqrt{\pi} n! 2^n}} H_n(\xi) e^{-\xi^2/2} \\ = &\left[\widehat{\widehat{E}} - (m + 1/2) \right] \sum_{n=0}^{\infty} \alpha_n \int_{-\infty}^{+\infty} d\xi \frac{1}{\sqrt{\sqrt{\pi} m! 2^m \sqrt{\pi} n! 2^n}} H_m(\xi) e^{-\xi^2/2} H_n(\xi) e^{-\xi^2/2} \end{aligned} \tag{4.85}$$

Introducing the function,

$$U_l(\xi) = \frac{1}{\sqrt{\sqrt{\pi} l! 2^l}} H_l(\xi) e^{-\xi^2/2} \tag{4.86}$$

Leads to

$$\beta \sum_{n=0}^{\infty} \alpha_n \langle U_m(\xi) | \xi^r | U_n(\xi) \rangle = \left[\widehat{\widetilde{E}} - (m + 1/2) \right] \sum_{n=0}^{\infty} \alpha_n \langle U_m(\xi) \big| U_n(\xi) \rangle$$

With respect to the fact that

$$\int_{-\infty}^{+\infty} d\xi \, U_m(\xi) \, U_n(\xi) = \delta_{mn} \tag{4.87}$$

we obtain

$$\langle U_m(\xi) \big| U_n(\xi) \rangle = \delta_{mn} \tag{4.88}$$

Therefore, we have

$$\beta \sum_{n=0}^{\infty} \alpha_n \langle U_m(\xi) \big| \xi^r \big| U_n(\xi) \rangle = \left[\widehat{\widetilde{E}} - (m + 1/2) \right] \sum_{n=0}^{\infty} \alpha_n \delta_{mn} \tag{4.89}$$

Using the expression for $U_m(\xi)$ and $U_n(\xi)$ according to (4.86), we have:

$$\langle U_m(\xi) \big| \xi^r \big| U_n(\xi) \rangle = \frac{1}{\sqrt{\sqrt{\pi} m! 2^m}} \frac{1}{\sqrt{\sqrt{\pi} n! 2^n}} \int_{-\infty}^{\infty} d\xi \, H_m(\xi) H_n(\xi) \xi^r e^{-\xi^2} \tag{4.90}$$

Preparatory Calculations:

$$H_m(\xi) = a_m\xi^m + a_{m-2}\xi^{m-2} + \cdots \tag{4.91a}$$

$$H_n(\xi) = b_n\xi^n + b_{n-2}\xi^{n-2} + b_{n-4}\xi^{n-4} + \cdots \tag{4.91b}$$

‘

Coefficients of $H_m(\xi)H_n(\xi)$ can be determined

$$\begin{aligned}
\text{Coefficient}\left\{H_m(\xi)H_n(\xi)\right\} &= \begin{bmatrix} a_m \\ a_{m-2} \\ \vdots \end{bmatrix} \begin{bmatrix} b_n & b_{n-2} & b_{n-4} & \dots \end{bmatrix} \\
&= \begin{bmatrix} a_m b_n & a_m b_{n-2} & a_m b_{n-4} & \dots \\ a_{m-2} b_n & a_{m-2} b_{n-2} & a_{m-2} b_{n-4} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \\
\text{Exponents}\left\{H_m(\xi)H_n(\xi)\right\} &= \begin{bmatrix} \xi^m \\ \xi^{m-2} \\ \vdots \end{bmatrix} \begin{bmatrix} \xi^n & \xi^{n-2} & \xi^{n-4} & \dots \end{bmatrix} \\
&= \begin{bmatrix} \xi^m\xi^n & \xi^m\xi^{n-2} & \xi^m\xi^{n-4} & \dots \\ \xi^{m-2}\xi^n & \xi^{m-2}\xi^{n-2} & \xi^{m-2}\xi^{n-4} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}
\end{aligned}$$

The following table provides the normalized Hermite polynomials for the first ten polynomials.

U_l	ξ^0	ξ^1	ξ^2	ξ^3	ξ^4	ξ^5	ξ^6	ξ^7	ξ^8	ξ^9
$U_0(\xi)$	0	0.7511	0	0	0	0	0	0	0	0
$U_1(\xi)$	0.3756	0	-0.1878	0	0	0	0	0	0	0
$U_2(\xi)$	0	0.1252	0	-0.1878	0	0	0	0	0	0
$U_3(\xi)$	0.0313	0	-0.0939	0	0.0235	0	0	0	0	0
$U_4(\xi)$	0	0.0063	0	-0.0313	0	0.0235	0	0	0	0
$U_5(\xi)$	0.001	0	-0.0078	0	0.0117	0	-0.002	0	0	0
$U_6(\xi)$	0	0.0001	0	-0.0016	0	0.0039	0	-0.002	0	0
$U_7(\xi)$	0	0	-0.0003	0	0.001	0	-0.001	0	0.0001	0
$U_8(\xi)$	0	0	0	0	0	0.0002	0	-0.0003	0	0.0001
$U_9(\xi)$	0	0	0	0	0	0	-0.0001	0	0.0001	0

Obviously we can write:

- If $l = 2k + 1$, then

$$U_l(\xi) = \sum_{i=0}^{k} \alpha_{2i+1} \xi^{2i+1}. \tag{4.92}$$

- If $l = 2k$, then

$$U_l(\xi) = \sum_{i=0}^{k} \alpha_{2i} \xi^{2i}. \tag{4.93}$$

Whenever the result of equation (4.90) is an even function, we have a nonvanishing outcome otherwise the outcome is zero. From the right-hand side of equation (4.90) we have four different cases where the outcome is an even function.

Note: We denote the m^{th} moment with respect to kernel $e^{-\xi^2}$ by I_m:

$$I_m = \int_{-\infty}^{+\infty} d\xi \xi^m e^{-\xi^2} \tag{4.94}$$

- When $r = 2r'$ (even), the following two conditions are valid

  Case 1: $m = 2m' + 1$ (odd) and $n = 2n' + 1$ (odd)

  $U_m(\xi)$ is an odd polynomial

  $U_n(\xi)$ is an odd polynomial

Multiplication of $U_m(\xi)$ and $U_n(\xi)$ results in an even function. Then the multiplication of an even function (x^r) by the resulting even function is itself an even function. Therefore, based on equation (4.105d) in Section 4.4 and equations(4.92) and (4.93), we can write the following result:

$$\beta \sum_{n=0}^{\infty} \alpha_n \int_{-\infty}^{+\infty} d\xi \sum_{k=0}^{m'} \alpha_{2k+1}\, \xi^{2k+1} \xi^{2r'} \sum_{l=0}^{n'} \alpha_{2l+1}\, \xi^{2l+1} e^{-\xi^2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m \tag{4.95}$$

Exchanging the order of summations and integration gives:

$$\beta \sum_{n=0}^{\infty} \sum_{k=0}^{m'} \sum_{l=0}^{n'} \alpha_n\, \alpha_{2k+1}\, \alpha_{2l+1} \int_{-\infty}^{+\infty} d\xi\, \xi^{2k+1}\, \xi^{2r'}\, \xi^{2l+1}\, e^{-\xi^2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m \tag{4.96}$$

In view of the equation (4.94), the integral in equation (4.96) is equal to $I_{2k+2l+2r'+2}$

$$\beta \sum_{n=0}^{\infty} \sum_{k=0}^{m'} \sum_{l=0}^{n'} \underbrace{\alpha_n\, \alpha_{2k+1}\, \alpha_{2l+1}}_{\alpha'_{n,2k+2,2l+1}} I_{2k+2l+2r'+2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m$$

Case 2: $m = 2m'$ (even)& $n = 2n'$ (even)

$U_m(\xi)$ is an even polynomial

$U_n(\xi)$ is an even polynomial

Multiplication of $U_m(x)$ and $U_n(\xi)$ results in an even function. Then the multiplication of an even function (ξ^r) by our even function is again an even function.

Therefore, based on equation (4.105d) in Section 4.4 and equations (4.92) and (4.93), we can have the following result:

$$\beta \sum_{n=0}^{\infty} \alpha_n \int_{-\infty}^{+\infty} d\xi \sum_{k=0}^{m'} \alpha_{2k}\, \xi^{2k} \xi^{2r'} \sum_{l=0}^{n'} \alpha_{2l}\, \xi^{2l} e^{-\xi^2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m \tag{4.97}$$

Therefore, exchanging the order of summations and integration gives:

$$\beta \sum_{n=0}^{\infty} \sum_{k=0}^{m'} \sum_{l=0}^{n'} \alpha_n\, \alpha_{2k}\, \alpha_{2l} \int_{-\infty}^{+\infty} d\xi\, \xi^{2k}\, \xi^{2r'}\, \xi^{2l}\, e^{-\xi^2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m$$

In view of the equation (4.94), the integral in equation (4.98) is $I_{2k+2l+2r'}$

$$\beta \sum_{n=0}^{\infty} \sum_{k=0}^{m'} \sum_{l=0}^{n'} \underbrace{\alpha_n\, \alpha_{2k}\, \alpha_{2l}}_{\alpha'_{2n,2k,2l}} I_{2k+2l+2r'} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m$$

- When $r = 2r' + 1$ (odd), the following two conditions are valid

Case 1: $m = 2m'$ (even)& $n = 2n' + 1$ (odd)

$U_m(\xi)$ is an even polynomial

$U_n(\xi)$ is an odd polynomial

Multiplication of $U_m(\xi)$ and $U_n(\xi)$ results in an odd function. Then multiplication of an odd function (ξ^r) by the resulting odd function is an even function. Therefore, based on equation (4.105d) in Section 4.4 and equations (4.92) and (4.93), we can result the following;

$$\beta\sum_{n=0}^{\infty}\alpha_n\int_{-\infty}^{+\infty}d\xi\sum_{k=0}^{m'}\alpha_{2k}\,\xi^{2k}\xi^{2r'+1}\sum_{l=0}^{n'}\alpha_{2l+1}\,\xi^{2l+1}e^{-\xi^2}=\left[\widehat{\widetilde{E}}-(m+1/2)\right]\alpha_m \tag{4.98}$$

Therefore,

$$\beta\sum_{n=0}^{\infty}\sum_{k=0}^{m'}\sum_{l=0}^{n'}\alpha_n\,\alpha_{2k}\,\alpha_{2l+1}\int_{-\infty}^{+\infty}d\xi\,\xi^{2k}\,\xi^{2r'+1}\,\xi^{2l+1}\,e^{-\xi^2}=\left[\widehat{\widetilde{E}}-(m+1/2)\right]\alpha_m \tag{4.99}$$

In view of the equation (4.94), the integral in equation (4.99) is $I_{2k+2l+2r'+2}$

$$\beta\sum_{n=0}^{\infty}\sum_{k=0}^{m'}\sum_{l=0}^{n'}\underbrace{\alpha_n\,\alpha_{2k+1}\,\alpha_{2l+1}}_{\alpha'_{n,2k+1,2l+1}}\,I_{2k+2l+2r'+2}=\left[\widehat{\widetilde{E}}-(m+1/2)\right]\alpha_m \tag{4.100}$$

Case 2: $m=2m'+1$ (odd)& $n=2n'$ (even)

$U_m(\xi)$ is an even polynomial

$U_n(\xi)$ is an odd polynomial

Multiplication of $U_m(\xi)$ and $U_n(\xi)$ results in an odd function. Then multiplication of an odd function (ξ^r) by the resulting odd function is an even function. Therefore, based on equation (4.105d) in Section 4.4 and equations (4.92) and (4.93), we can result the following;

$$\beta \sum_{n=0}^{\infty} \alpha_n \int_{-\infty}^{+\infty} d\xi \sum_{k=0}^{m'} \alpha_{2k+1}\, \xi^{2k+1} \xi^{2r'+1} \sum_{l=0}^{n'} \alpha_{2l}\, \xi^{2l} e^{-\xi^2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m \tag{4.101}$$

Therefore,

$$\beta \sum_{n=0}^{\infty} \sum_{k=0}^{m'} \sum_{l=0}^{n'} \alpha_n\, \alpha_{2k+1}\, \alpha_{2l} \int_{-\infty}^{+\infty} d\xi\, \xi^{2k+1}\, \xi^{2r'+1}\, \xi^{2l}\, e^{-\xi^2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m \tag{4.102}$$

In view of the equation (4.94), the integral in equation (4.102) is $I_{2k+2l+2r'+2}$

$$\beta \sum_{n=0}^{\infty} \sum_{k=0}^{m'} \sum_{l=0}^{n'} \underbrace{\alpha_n\, \alpha_{2k+1}\, \alpha_{2l}}_{\alpha'_{n,2k+1,2l}} I_{2k+2l+2r'+2} = \left[\widehat{\widehat{E}} - (m+1/2)\right] \alpha_m \tag{4.103}$$

I_{2l} can be calculated from equation (4.121) in Section 4.4.

4.4 Development of a Recursion Formula for the Calculation of $I_m(\xi)$

This section as it is used in our calculations extensively is in order to find out the value of I's.

This section is devoted to the calculation of the integrals which appear in the evaluation of interaction terms, $< U_m(\xi)|\xi^r|U_n(\xi) >$, i.e.,

$$I_m = \int_{-\infty}^{+\infty} d\xi \, p_m(\xi) \, e^{-\xi^2}. \tag{4.104}$$

Observe that we have the following results:

$$\begin{aligned}
I_0 &= \int_{-\infty}^{+\infty} d\xi \, e^{-\xi^2} && (4.105a)\\
I_1 &= \int_{-\infty}^{+\infty} d\xi \, \xi \, e^{-\xi^2} = 0 && (4.105b)\\
I_2 &= \int_{-\infty}^{+\infty} d\xi \, \xi^2 \, e^{-\xi^2} && (4.105c)\\
I_{2l+1} &= \int_{-\infty}^{+\infty} d\xi \, \xi^{2l+1} \, e^{-\xi^2} = 0 && (4.105d)\\
I_{2l} &= \int_{-\infty}^{+\infty} d\xi \, \xi^{2l} \, e^{-\xi^2} && (4.105e)
\end{aligned}$$

Furthermore, we have

$$\int_{-\infty}^{+\infty} d\xi \, e^{-\xi^2} = \sqrt{\pi}. \tag{4.106}$$

Based on (4.106) we obtain the values for $I_{2l}(l \in N)$ as follows.

$$\begin{aligned}
I_2 &= 2 \int_0^{\infty} d\xi \, \xi^2 \, e^{-\xi^2} \\
&= 2 \left\{ \frac{\xi^3}{3} \, e^{-\xi^2} \Big|_0^{\infty} - \int_0^{+\infty} d\xi \, \frac{\xi^3}{3} \, (-2\xi) \, e^{-\xi^2} \right\} && (4.107)
\end{aligned}$$

Considering the fact that

$$\frac{\xi^3}{3}\, e^{-\xi^2}\Big|_0^\infty = 0 \tag{4.108}$$

We have,

$$\begin{aligned} I_2 &= \frac{4}{3}\int_0^{+\infty} d\xi\, \xi^4\, e^{-\xi^2} \\ &= \frac{2}{3}\left\{ 2\int_0^{+\infty} d\xi\, \xi^4\, e^{-\xi^2} \right\} \\ &= \frac{2}{3}\, I_4 \end{aligned} \tag{4.109}$$

Or, alternatively,

$$I_4 = \frac{3}{2}\, I_2 \tag{4.110}$$

Thus, reducing the calculation of I_4 to I_2.

$$\begin{aligned} I_4 &= 2\int_0^{+\infty} d\xi\, \xi^4\, e^{-\xi^2} \\ &= 2\left\{ \frac{\xi^5}{5}\, e^{-\xi^2}\Big|_0^\infty - \int_0^{+\infty} d\xi\, \frac{\xi^5}{5}\, (-2\xi)\, e^{-\xi^2} \right\} \qquad (4.111) \\ &= \frac{4}{5}\int_0^{+\infty} d\xi\, \xi^6\, e^{-\xi^2} \\ &= \frac{2}{5}\left\{ 2\int_0^{+\infty} d\xi\, \xi^6\, e^{-\xi^2} \right\} \\ &= \frac{2}{5}\, I_6 \qquad (4.112) \end{aligned}$$

Or, alternatively,

$$I_6 = \frac{5}{2} I_4 \tag{4.113}$$

Thus, reducing the calculation of I_6 to I_4.

Based on equations (4.110) and (4.114) we have:

$$I_6 = \frac{5}{2}\frac{3}{2} I_2 \tag{4.114}$$

Similarly we can show that

$$I_{2l} = \frac{2l-1}{2} I_{2l-2} \tag{4.115}$$

Or, alternatively,

$$I_{2l-2} = \frac{2}{2l-1} I_{2l} \tag{4.116}$$

Finally I_{2l} can be expressed in terms of I_{2l+2}:

$$\begin{aligned} I_{2l} &= \int_{-\infty}^{+\infty} d\xi\, \xi^{2l}\, e^{-\xi^2} \\ &= 2\int_{0}^{+\infty} d\xi\, \xi^{2l}\, e^{-\xi^2} \\ &= 2\left\{ \frac{\xi^{2l+1}}{2l+1}\, e^{-\xi^2}\Big|_0^{\infty} - \frac{1}{2l+1}\int_0^{+\infty} d\xi\, (-2\xi)\, \xi^{2l+1}\, e^{-\xi^2} \right\} \\ &= \frac{2}{2l+1}\, 2\int_0^{+\infty} d\xi\, \xi^{2l+2}\, e^{-\xi^2} \\ &= \frac{2}{2l+1}\, I_{2l+2} \end{aligned} \tag{4.117}$$

Thus,

$$I_{2l} = \frac{2}{2l+1}\, I_{2l+2} \tag{4.118}$$

Or, similarly,

$$I_{2l+2} = \frac{2}{2l+3}\, I_{2l+4}. \tag{4.119}$$

The following reformulations are self explanatory:

$$\begin{aligned} I_{2l+4} &= \frac{2l+3}{2}\, I_{2l+2} \\ &= \frac{2l+3}{2}\, \frac{2l+1}{2}\, I_{2l} \end{aligned} \tag{4.120}$$

Consequently by induction we can write:

$$I_{2l} = \frac{1}{2^l}\prod_{l=0}^{l-1}(2l+1)I_0 \tag{4.121}$$

Therefore, we have been able to reduce the calculation of I_{2l} to I_0 with I_0 being equal to $\sqrt{\pi}$.

This convenient recursion formula for the calculation of I_{2l} has extensively used in our calculation significantly facilitating the numerical procedures.

4.5 An Observation How Matlab Presents the Calculated Eigenvalues and Eigenvectors

In numerical calculation of perturbed harmonic oscillator problem with Matlab an important observation was made. The observation was made in relation to the solution of eigenequations. The ''problem'' occurs whenever the dimension of the system matrix exceeds 5. In case of r being an even number, the matrix exhibits the following symmetry pattern.

$$\left\{\begin{bmatrix} A_{11} & 0 & A_{13} & 0 \\ 0 & A_{22} & 0 & A_{24} \\ A_{31} & 0 & A_{33} & 0 \\ 0 & A_{42} & 0 & A_{44} \end{bmatrix} + \begin{bmatrix} d_{11} & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & d_{44} \end{bmatrix}\right\} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = \lambda \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} \tag{4.122}$$

The pattern of the A-matrix suggests the following ''obvious'' decomposition of the A and the diagonal matrices into the matrices P, Q and E, F, respectively.

$$\left\{ \underbrace{\begin{bmatrix} A_{11} & 0 & A_{13} & 0 \\ 0 & 0 & 0 & 0 \\ A_{31} & 0 & A_{33} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{P} + \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & A_{22} & 0 & A_{24} \\ 0 & 0 & 0 & 0 \\ 0 & A_{42} & 0 & A_{44} \end{bmatrix}}_{Q} \right.$$
$$\left. + \underbrace{\begin{bmatrix} d_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}}_{E} + \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{44} \end{bmatrix}}_{F} \right\}$$
$$+ \left\{ \begin{bmatrix} \alpha_1 \\ 0 \\ \alpha_3 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \alpha_2 \\ 0 \\ \alpha_4 \end{bmatrix} \right\} = \lambda \left\{ \underbrace{\begin{bmatrix} \alpha_1 \\ 0 \\ \alpha_3 \\ 0 \end{bmatrix}}_{a} + \underbrace{\begin{bmatrix} 0 \\ \alpha_2 \\ 0 \\ \alpha_4 \end{bmatrix}}_{b} \right\} \tag{4.123}$$

therefore, we obtain:

$$[P + Q + E + F][a + b] = \lambda[a + b] \tag{4.124a}$$

$$Pa + 0 + 0 + Qb + Ea + Fb = \lambda a + \lambda b \tag{4.124b}$$

based on equation (4.124a) and (4.124b)

$$\begin{cases} Pa + Ea = \lambda a \\ Qb + Fb = \lambda b \end{cases} \Longrightarrow \begin{cases} \underbrace{(P + E)}_{T} a = \lambda a \\ \underbrace{(Q + F)}_{S} b = \lambda b \end{cases}$$

the above equations show that this system can be decoupled and diagonal matrix $D = E + F$ can be absorbed into A.

On the other hand, when r is odd we have

$$\left\{ \begin{bmatrix} 0 & A_{12} & 0 & A_{14} \\ A_{21} & 0 & A_{23} & 0 \\ 0 & A_{32} & 0 & A_{34} \\ A_{41} & 0 & A_{43} & 0 \end{bmatrix} + \begin{bmatrix} d_{11} & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & d_{44} \end{bmatrix} \right\} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = \lambda \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} \tag{4.125}$$

By decomposing the matrices A and D in the obvious form:

$$\begin{aligned} &\left\{ \begin{bmatrix} 0 & A_{12} & 0 & A_{14} \\ 0 & 0 & 0 & 0 \\ 0 & A_{32} & 0 & A_{34} \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ A_{21} & 0 & A_{23} & 0 \\ 0 & 0 & 0 & 0 \\ A_{41} & 0 & A_{43} & 0 \end{bmatrix} \right. \\ &\left. + \begin{bmatrix} d_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{44} \end{bmatrix} \right\} \\ &+ \left\{ \begin{bmatrix} \alpha_1 \\ 0 \\ \alpha_3 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \alpha_2 \\ 0 \\ \alpha_4 \end{bmatrix} \right\} = \lambda \left\{ \begin{bmatrix} \alpha_1 \\ 0 \\ \alpha_3 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \alpha_2 \\ 0 \\ \alpha_4 \end{bmatrix} \right\} \end{aligned} \tag{4.126}$$

we obtain

$$[P + Q + E + F][a + b] = \lambda[a + b] \tag{4.127a}$$

$$0 + Pb + Qb + 0 + Ea + Fb = \lambda a + \lambda b \tag{4.127b}$$

where the zero indicates a 4-by-4 null matrix. Taking into account the structure of the matrices P, Q, E and F and the structure of the vectors a and b, we realize the equation (4.127a) and (4.127b) can be written in the form.

$$\begin{cases} Pb + Ea = \lambda a \\ \\ Qa + Fb = \lambda b \end{cases} \Longrightarrow \begin{cases} Pb = (\lambda I - E)a \\ \\ Qa = (\lambda I - F)b \end{cases}$$

However, in this case the original system-matrix $A + D$ cannot be decoupled and the diagonal matrix D cannot be absorbed into the matrices P and Q.

$\beta_r x^r$ with r being even As we learned from this analysis in cases where r in $\beta_r x^r$ is an even number the discretized version of the problem which leads to a system matrix can be decoupled into eigenvalue problem. As rule the eigenvalues are arranged in increasing order with their corresponding eigenvectors arranged in the resulting eigenvector matrix. In carrying out the evaluation of the eigenpairs by Matlab two cases may happen: N_{dim} the dimension of the system matrix less equal or larger than 5, as we have observed.

Case 1: the system-matrix A_{mn} for $\eta = 100$ and $N_{dim} = 5$ for r=2 is the following $(N_{dim} + 1) \times (N_{dim} + 1)$ matrix:

$$\begin{bmatrix} 50.5000 & 0 & 0.2500 & 0 & 0 & 0 \\ 0 & 150.7500 & 0 & 0.1250 & 0 & 0 \\ 0.2500 & 0 & 250.3125 & 0 & 0.0313 & 0 \\ 0 & 0.1250 & 0 & 350.0729 & 0 & 0.0052 \\ 0 & 0 & 0.0313 & 0 & 450.0117 & 0 \\ 0 & 0 & 0 & 0.0052 & 0 & 550.0014 \end{bmatrix}$$

Eigenvalues of A_{mn} are,

$$\begin{bmatrix} 50.4997 & 0 & 0 & 0 & 0 & 0 \\ 0 & 150.7499 & 0 & 0 & 0 & 0 \\ 0 & 0 & 250.3128 & 0 & 0 & 0 \\ 0 & 0 & 0 & 350.0730 & 0 & 0 \\ 0 & 0 & 0 & 0 & 450.0117 & 0 \\ 0 & 0 & 0 & 0 & 0 & 550.0014 \end{bmatrix}$$

with the corresponding eigenvectors of A_{mn}

$$\begin{bmatrix} 1.0000 & 0.0000 & -0.0013 & -0.0000 & -0.0000 & 0.0000 \\ -0.0000 & 1.0000 & 0.0000 & 0.0006 & -0.0000 & 0.0000 \\ -0.0013 & 0.0000 & -1.0000 & -0.0000 & -0.0002 & 0.0000 \\ -0.0000 & -0.0006 & -0.0000 & 1.0000 & -0.0000 & 0.0000 \\ 0.0000 & -0.0000 & 0.0002 & -0.0000 & -1.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & -0.0000 & 0.0000 & 1.0000 \end{bmatrix}$$

We recognize that the eigenvalues appear in the increasing order as we would expect.

Case 2: Next, we consider the same problem ($\eta = 100$, $r = 2$), however, this time with $N_{dim} = 8$ instead of $N_{dim} = 5$. We obtain the following result:

the $(8 + 1) \times (8 + 1)$ system-matrix A has the following form:

$$\begin{bmatrix} 50.5000 & 0 & 0.2500 & 0 & -0.0000 & 0 & 0.0000 & 0 & -0.0000 \\ 0 & 150.7500 & 0 & 0.1250 & 0 & 0.0000 & 0 & -0.0000 & 0 \\ 0.2500 & 0 & 250.3125 & 0 & 0.0313 & 0 & 0 & 0 & -0.0000 \\ 0 & 0.1250 & 0 & 350.0729 & 0 & 0.0052 & 0 & -0.0000 & 0 \\ -0.0000 & 0 & 0.0313 & 0 & 450.0117 & 0 & 0.0007 & 0 & 0.0000 \\ 0 & 0.0000 & 0 & 0.0052 & 0 & 550.0014 & 0 & 0.0001 & 0 \\ 0.0000 & 0 & 0.0000 & 0 & 0.0007 & 0 & 650.0001 & 0 & 0.0000 \\ 0 & -0.0000 & 0 & -0.0000 & 0 & 0.0001 & 0 & 750.0000 & 0 \\ -0.0000 & 0 & -0.0000 & 0 & 0 & 0 & 0.0000 & 0 & 850.0000 \end{bmatrix}$$

for the eigenvalues of A_{mn} we obtain:

$$\begin{bmatrix} 50.4997 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 250.3128 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 450.0117 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 650.0001 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 850.0000 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 150.7499 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 350.0730 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 550.0014 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 750.0000 \end{bmatrix}$$

with the corresponding eigenvectors of A_{mn}

$$\begin{bmatrix} -1.0000 & 0.0013 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0.0006 & 0 & 0 \\ 0.0013 & 1 & -0.0002 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0006 & 1 & 0 & 0 \\ 0 & -0.0002 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Comparing the two eigenvalue matrices, we realize that the eigenvalues do not appear in increasing order, but rather seemingly in a mix order. However, a closer scrutiny of the eigenvalues reveals the fact that the first five eigenvalues corresponds to the S matrix and the remaining four eigenvalues correspond to the T matrix introduced earlier this observation is of value since ordinarily it is assumed that the eigenvalues appear in increasing order with larger eigenvalue being calculated with less accuracy.

Summary: The composition $A \longrightarrow S + T$ carried out by Matlab automatically, explains the apparent rearrangement of the eigenvalues in the eigenvalue matrix above.

In case of odd powers, there is no such a symmetry. Therefore, we do not have any decoupling of matrix. However, when the matrix dimension increases the off-diagonal elements approach zero. This property may cause decoupling toward the end of eigenvalue and eigenvector matrices where off-diagonals are nearly zero.

4.6 Summary

An easy-to-implement method for the determination of eigenpairs of monomially perturbed harmonic oscillators has been purposed. The method is based on using the ideal unperturbed harmonic oscillator as an auxiliary problem. We have shown that our solution concept leads to an algebraic system for the determination of unknowns of the problem with closed-form formula for the arising matrix elements.

Chapter 5

Numerical Results

5.1 Numerical Results

In this chapter we apply our theory, developed and discussed in Chapter 4, to a large number of problems and present the numerical results graphically. The results shows that the proposed formalism applies to perturbed harmonic oscillators with arbitrary monomials $\beta_r x^r$ with arbitrarily high integer-valued exponents r, irrespectively, of r being even or odd.

To obtain numerical results we first truncate the sum in (5.1) by taking into account $N+1$ terms only ($n = 0 \cdots N$). Furthermore, we introduced $\widetilde{\widetilde{E}} = \widehat{\widetilde{E}}/\beta$ to obtain:

$$\sum_{n=0}^{N} \alpha_n \int_{-\infty}^{+\infty} d\xi \, U_m(\xi) \xi^r \, U_n(\xi) = [\widetilde{\widetilde{E}} - (m + \frac{1}{2})\eta]\alpha_m \tag{5.1}$$

For a given m (5.1) represents one equation for the unknown expansion coefficients $\{\alpha_0, \cdots, \alpha_N\}$. Let m vary from 0 to N, then we obtain an $(N+1) \times (N+1)$ eigenvalue equation. The eigenvalues and corresponding eigenvectors of the resulting eigensystem

are the desired $\overset{\approx}{\overset{\approx}{E}}_k$ and the associated eigenvectors, which are represented as the column vectors of the matrix $\{\alpha_{lk}\big|l = 0, \cdots, N; k = 0, \cdots, N\}$.

Next, we consider graphs for r being even, respectively, odd.

5.1.1 Monomial Perturbations of Even Order ($r = 2r'$)

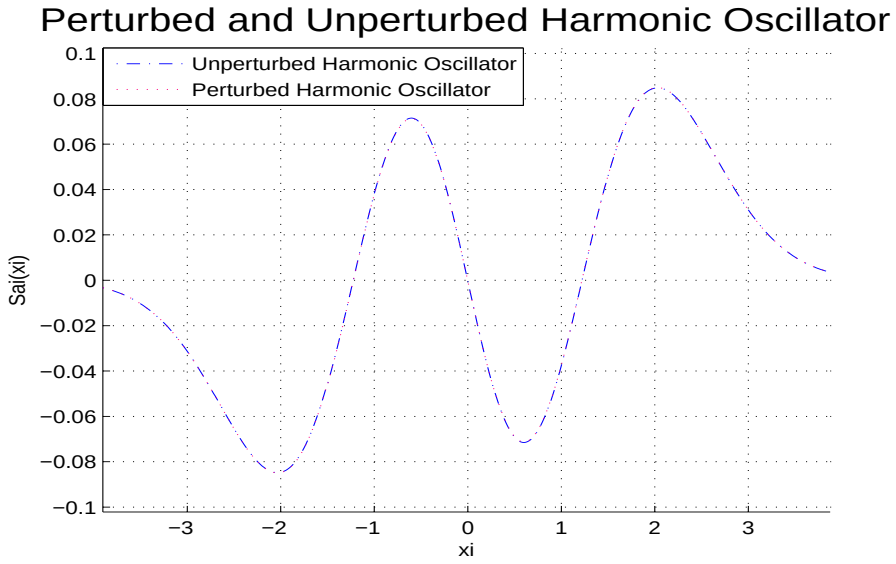

Figure 5.1: N_{dim}=8, $\eta = 100$, $r = 2$, 3^{rd} eigensolution of Perturbed Harmonic Oscillator

In figure (5.1), we chose η to be 100 which corresponds to a very small perturbation. This result from the fact that $\eta = 1/\beta$ with β being the perturbation parameter. β appearing as βx^r in the Schrödinger equation. As we can see for a small perturbation, perturbed and unperturbed harmonic oscillator have nearly indistinguishable eigenfunctions ψ and $\widetilde{\psi}$.

We could observe that for small values of the perturbation parameter β (large values of η) the graphs for perturbed and unperturbed eigenfunctions remain nearly indistinguishable. This is comforting since this property ensures rapid convergence in the

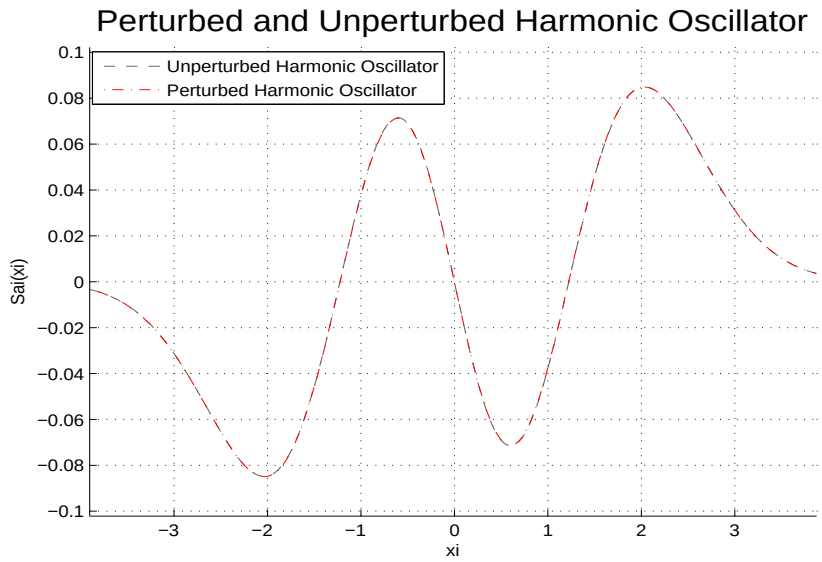

Figure 5.2: N_{dim}=5, $\eta = 100$, $r = 2$, 3rd eigensolution of Perturbed Harmonic Oscillator

series expansions for the perturbed solution. We examined this behavior by increasing the N_{dim} up to 16.

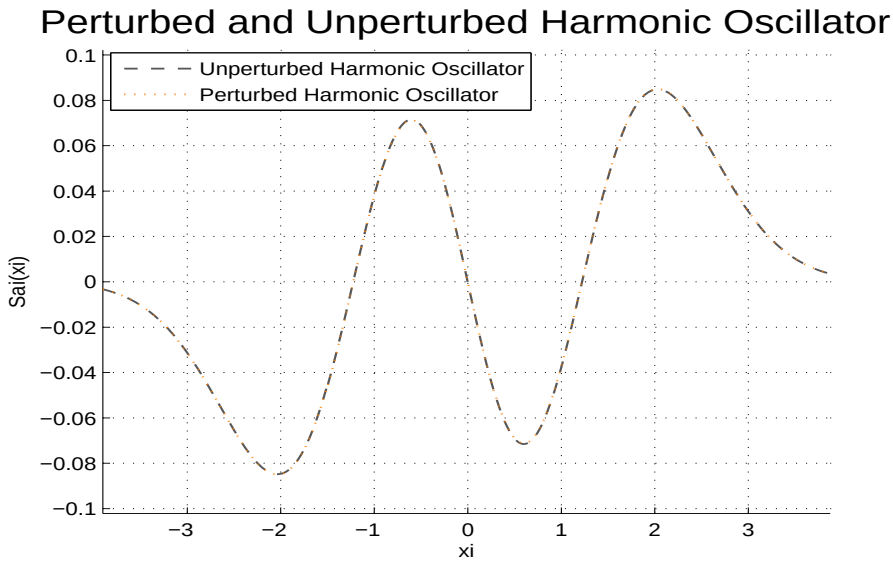

Figure 5.3: N_{dim}=16, $\eta = 100$, $r = 2$, 3rd eigensolution of Perturbed Harmonic Oscillator

In Figure (5.3), by increasing the perturbation (reducing $\eta = 1/\beta$ to 10) we observe slight difference between the perturbed and unperturbed solutions which can be rec-

ognized in the corresponding graphs.

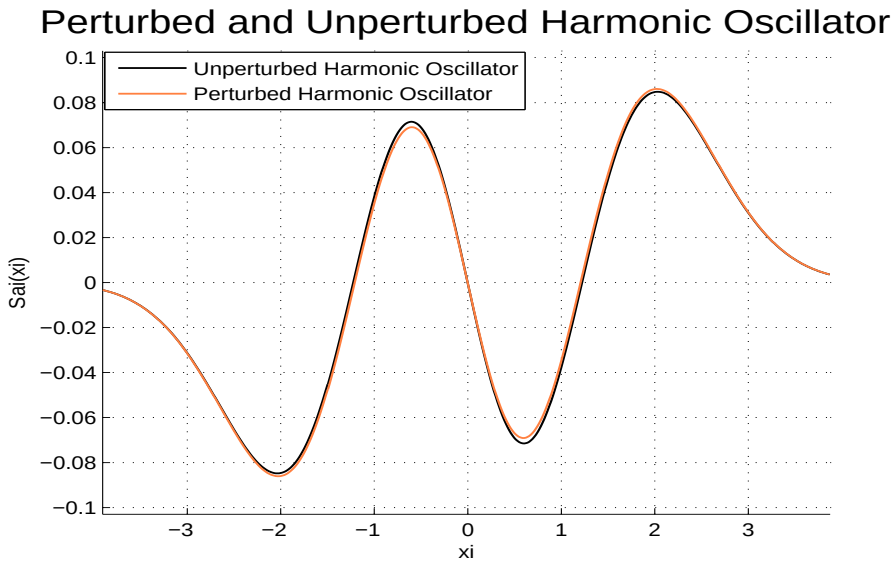

Figure 5.4: N_{dim}=5, $\eta = 10$, $r = 2$, 3rd eigensolution of Perturbed Harmonic Oscillator

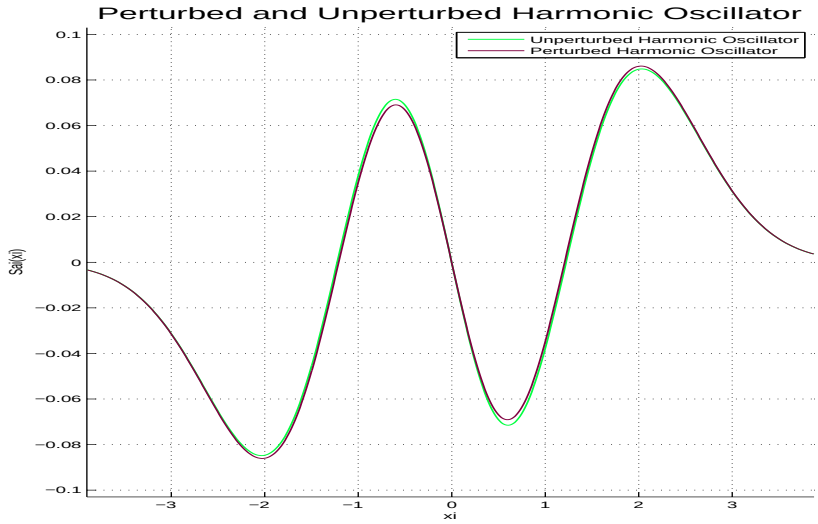

Figure 5.5: N_{dim}=10, $\eta = 10$, $r = 2$, 3rd eigensolution of Perturbed Harmonic Oscillator

In Figure (5.5), the case with $\eta = 10$ we have larger perturbation for various matrix dimensions.

When η is one, the magnitude of perturbation is large, and perturbation can be seen

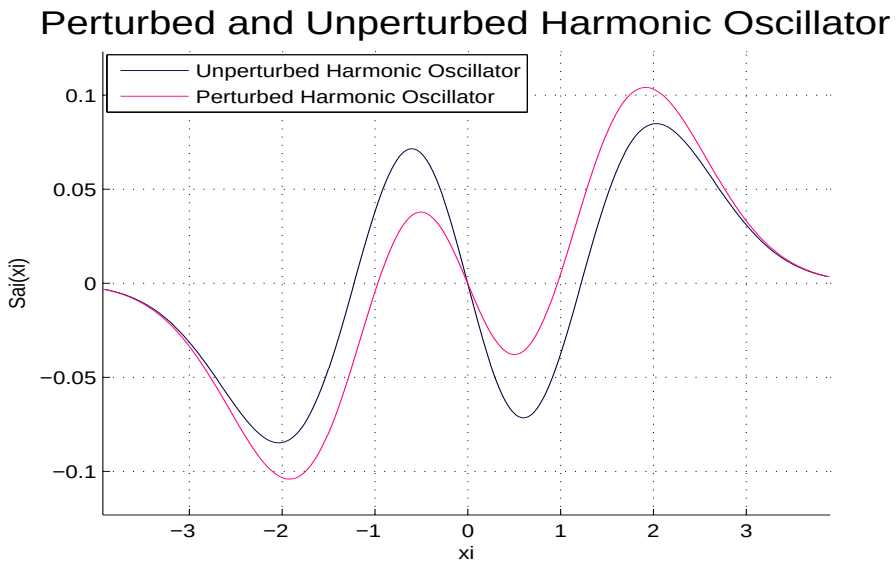

Figure 5.6: N_{dim}=8, $\eta = 1$, $r = 2$, 3rd eigensolution of Perturbed Harmonic Oscillator

clearly.

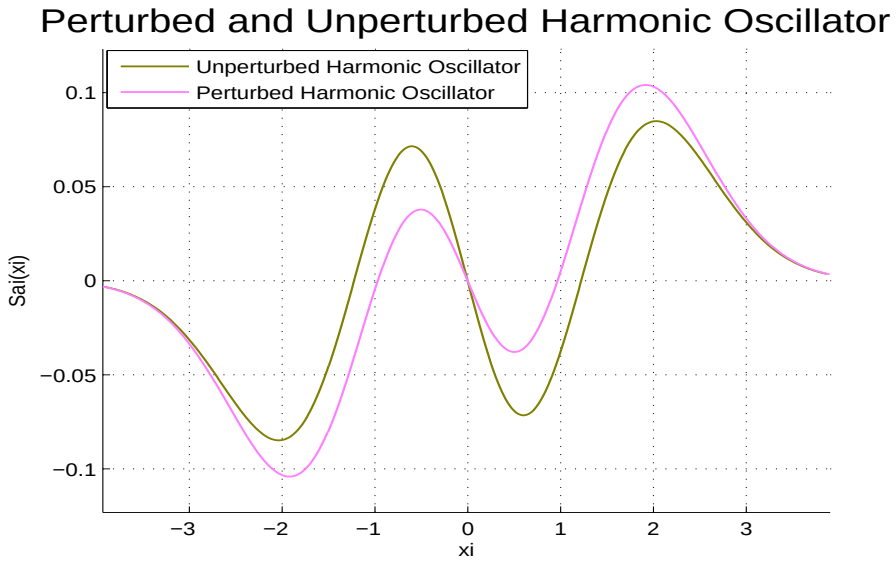

Figure 5.7: N_{dim}=5, $\eta = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

In Figures (5.6) and (5.7) η is equal to 1 ($\beta = 1$). Again rapid convergence manifests itself in the fact that, irrespective of the chosen matrix dimensions, we obtain virtually the same result for the perturbed eigenfunctions for the same degree of perturbation.

By analyzing graphs, eigenvalues and eigenvectors of matrix dimension five and eight in detail, we can see disorientation of their eigenvalues and eigenvectors. This is because of the decoupling of Matlab for calculating these values for matrix dimension of more than five. This is an issue for even-function perturbation mostly, as we have some sort of symmetry in A_{mn} matrix.

The symbolic (automatic) decoupling of the system-matrices for even r are demonstrated here for $N_{dim} = 5$ and $N_{dim} = 8$, respectively. The graphical representation of the eigenvalues clearly demonstrate the matrix decoupling and explains the apparent violation of monotically increasing of the successive eigenvalues.

$$A_{mn} = \begin{bmatrix} 1 & 0 & 0.25 & 0 & 0 & 0 \\ 0 & 2.25 & 0 & 0.125 & 0 & 0 \\ 0.25 & 0 & 2.812 & 0 & 0.0313 & 0 \\ 0 & 0.125 & 0 & 3.572 & 0 & 0.0052 \\ 0 & 0 & 0.0313 & 0 & 4.5117 & 0 \\ 0 & 0 & 0 & 0.0052 & 0 & 5.5014 \end{bmatrix}$$

Eigenvalues and the corresponding eigenvectors for $N_{dim} = 5$ with $\eta = 1$ and r=2 are calculated next.

Eigenvalues:

$$\begin{bmatrix} 0.9661 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.2383 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.8458 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.5846 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.5123 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5.5014 \end{bmatrix}$$

The corresponding eigenvectors:

$$\begin{bmatrix} 0.991 & 0 & -0.1342 & 0 & -0.0013 & 0 \\ 0 & 0.9956 & 0 & 0.0933 & 0 & 0.0001 \\ -0.1342 & 0 & -0.9908 & 0 & -0.0186 & 0 \\ 0 & -0.0933 & 0 & 0.9956 & 0 & 0.0027 \\ 0.0012 & 0 & 0.0186 & 0 & -0.9998 & 0 \\ 0 & 0.0001 & 0 & -0.0027 & 0 & 1 \end{bmatrix}$$

The above six eigenvalues are graphically represented in Figure (5.8).

As expected the eigenvalues appear in ascending order corresponding from the 0^{th} to the 5^{th} perturbed eigenfunctions.

A_{mn} for $N_{dim} = 8$ with the same perturbation strength ($\eta = 1$) as in the previous case.

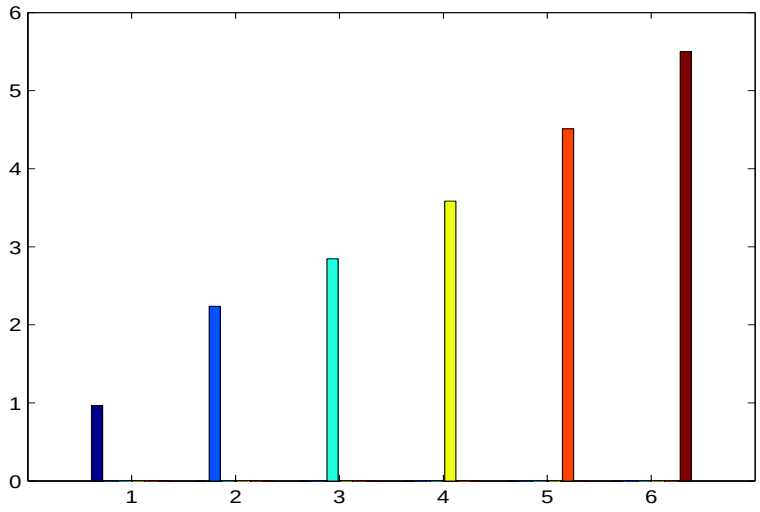

Figure 5.8: The graph of the Eigenvalues for N_{dim}=5, $r = 2$, $\eta = 1$

$$A_{mn} = \begin{bmatrix} 1 & 0 & 0.25 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.25 & 0 & 0.1250 & 0 & 0 & 0 & 0 & 0 \\ 0.25 & 0 & 2.812 & 0 & 0.0313 & 0 & 0 & 0 & 0 \\ 0 & 0.125 & 0 & 3.5729 & 0 & 0.0052 & 0 & 0 & 0 \\ 0 & 0 & 0.031 & 0 & 4.5117 & 0 & 0.0007 & 0 & 0 \\ 0 & 0 & 0 & 0.0052 & 0 & 5.5014 & 0 & 0.0001 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6.5001 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8.5 \end{bmatrix}$$

Eigenvalue and eigenvector for $N_{dim} = 8$ corresponding to a ‘‘perturbation’’ $\beta\xi^2$ is shown next.

Eigenvalues:

$$\begin{bmatrix} 0.9661 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.8458 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4.5123 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6.5001 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.2383 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3.5846 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.5014 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.5 \end{bmatrix}$$

The corresponding eigenvectors:

$$\begin{bmatrix} 0.991 & -0.1342 & 0.0013 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.9956 & 0.0933 & -0.0001 & 0 \\ -0.1342 & -0.9908 & 0.0186 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0933 & 0.9956 & -0.0027 & 0 \\ 0.0012 & 0.0186 & 0.9998 & 0.0003 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.0001 & -0.0027 & -1 & 0 \\ 0 & 0 & -0.0003 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The above are the eigenvalues and the corresponding eigenvectors for $N_{dim} = 8$. It is shown that the eigenvalues appear misplaced (not in monotically increasing order). However, this misplacement follows a recognizable pattern. Obviously wherever the

eigenvalues are shifted to another column its corresponding eigenvector is shifted to the same column.

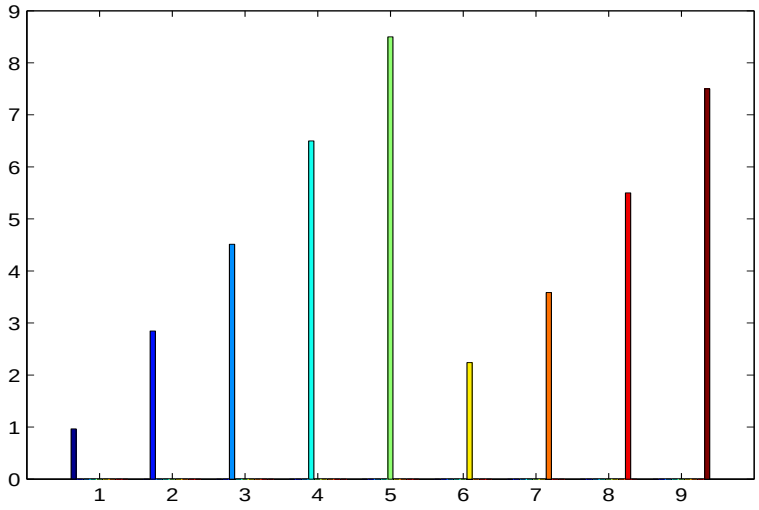

Figure 5.9: The graph of the Eigenvalues for N_{dim}=8, $r = 2$, $\eta = 1$

Therefore, in order to compare the perturbed solution associated with the unperturbed one, we should figure out which solution in the eigenvalue matrix we are looking for. For instance, in the case $N_{dim} = 8$ the 3^{rd} solution appears in column seven. That is, if we want to compare 3^{rd} unperturbed and perturbed solutions, comparison should be made between 4^{th} column of the ψ matrix and the 7^{th} column of the $\widetilde{\psi}$ matrix. It took us pains to decipher that Matlab decomposes matrices (in eigenvalue problem) whenever it is possible to do so. Our conclusion is the observing the monotonicity of the order of eigenvalues in a good check to recognize this decomposition. Or, alternatively, we can order the eigenvalues in increasing order (with reordering their corresponding eigenvectors). Then, no misinterpretation can take place.

The following graphs show a fix N_{dim} with varying exponents r for even-function mono-

mials.

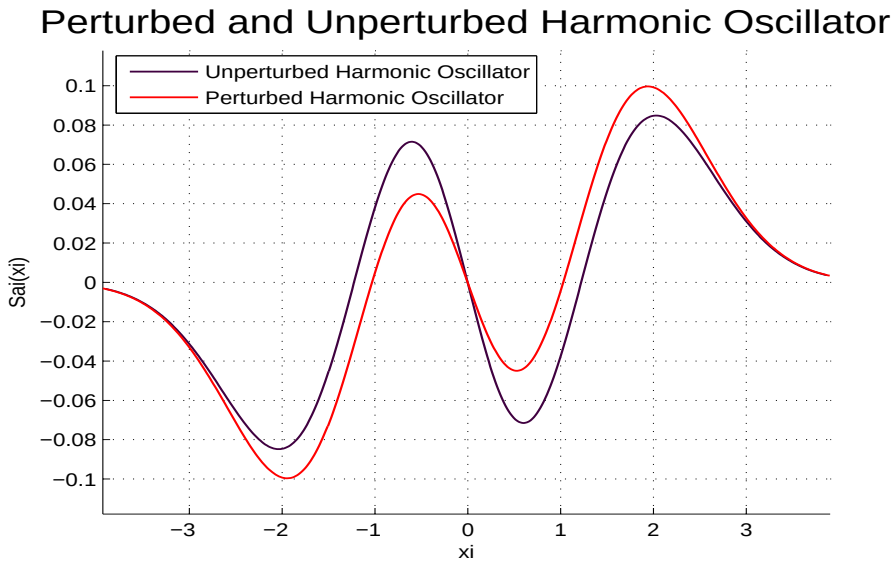

Figure 5.10: N_{dim}=9, $\eta = 5$, $r = 4$, 3rd eigensolution of Perturbed Harmonic Oscillator

The perturbative term for the above plot is $5\hbar\omega\xi^4$. Consequently, the magnitude of the perturbation is $5\hbar\omega$ which corresponds to $\beta = 5$. Figure (5.11) compares the 3rd solution of the perturbed solution with the corresponding eigenfunction of the unperturbed harmonic oscillator.

In this figure (5.11), we have even-order perturbation ($5\xi^6$) but perturbation order is different from Figure (5.10). In order to find the third perturbed solution in Figure (5.11) we should look for the corresponding perturbed solution in eigenvalue matrix.

In the above plot (5.12), matrix dimension is different, but we are comparing the same solution with the same perturbation term.

In the next section we will focus on the monomial perturbation of off order.

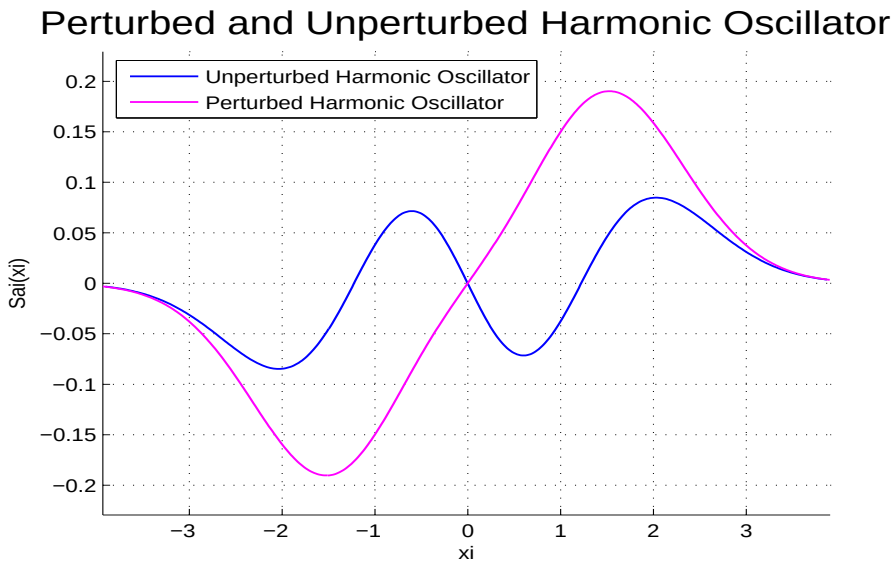

Figure 5.11: N_{dim}=9, $\eta = 5$, $r = 6$, 3rd eigensolution of Perturbed Harmonic Oscillator

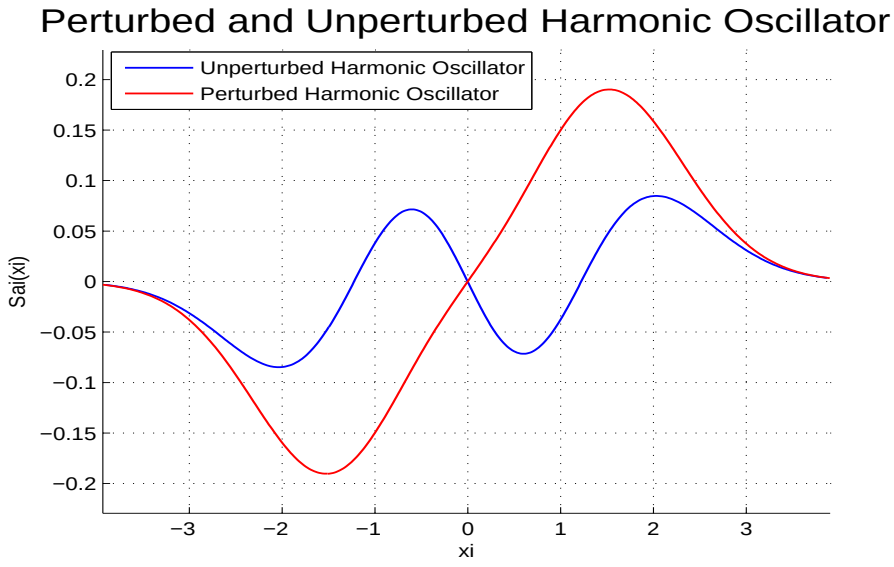

Figure 5.12: N_{dim}=5, $\eta = 5$, $r = 6$, 3rd eigensolution of Perturbed Harmonic Oscillator

5.1.2 Monomial Perturbations of Odd Order $(r = 2r' + 1)$

For r being an odd number we have the following pattern for the system-matrix $A_{mn}^{2r'+1}$:

$$A_{mn}^{(2r'+1)} = \begin{bmatrix} d_{11} & A_{12} & 0 & A_{14} \\ A_{21} & d_{22} & A_{23} & 0 \\ 0 & A_{32} & d_{33} & A_{34} \\ A_{41} & 0 & A_{43} & d_{44} \end{bmatrix}$$

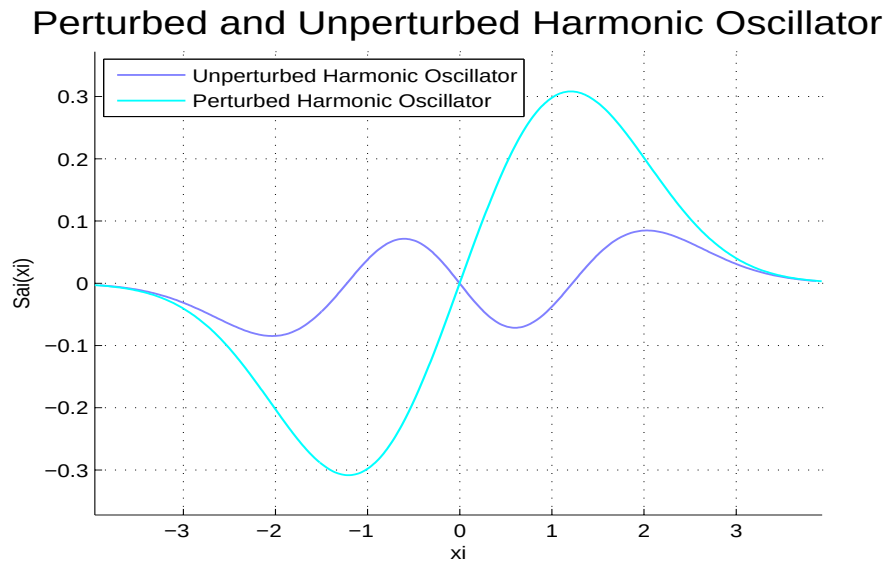

Figure 5.13: N_{dim}=9, $\eta = 5$, $r = 8$, 3rd eigensolution of Perturbed Harmonic Oscillator

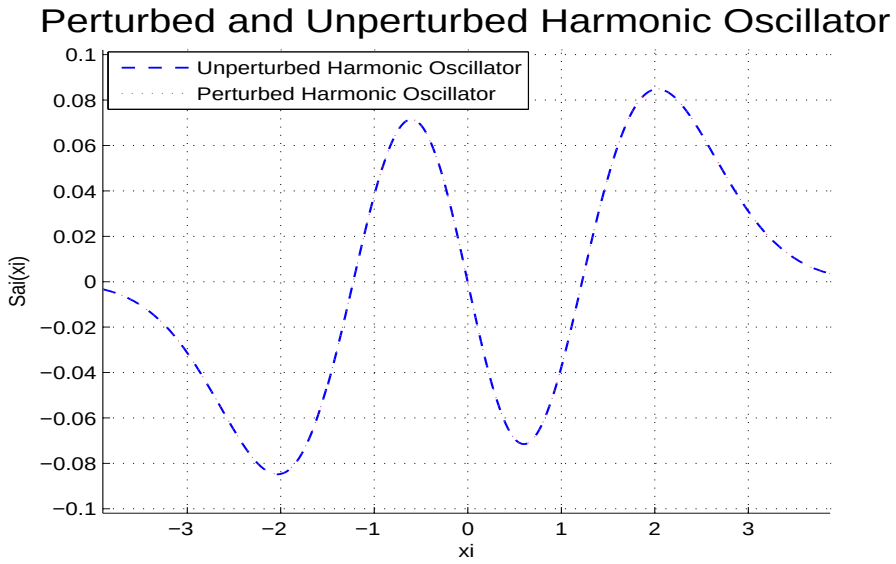

Figure 5.14: N_{dim}=8, $\eta = 100$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

Figure (5.14) is similar to Figure (5.1). The only difference between them is the fact that the latter figure is for perturbation power one, which signifies a linear perturbation. The matrix dimension and perturbation coefficient are held to be the same.

Similar to the previous figure, this figure (5.15) corresponds to Figure (5.2) with dif-

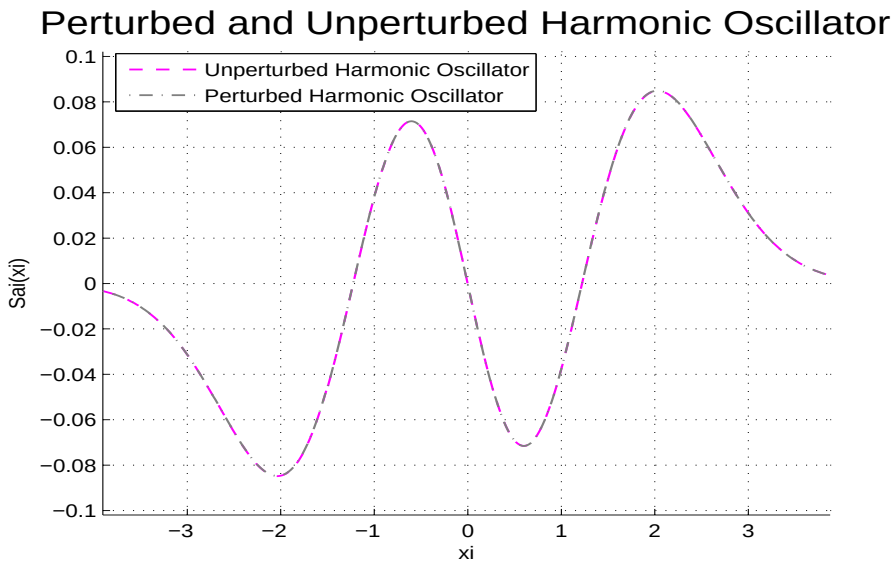

Figure 5.15: N_{dim}=5, $\eta = 100$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

ferent perturbation power and a very small magnitude of perturbation.

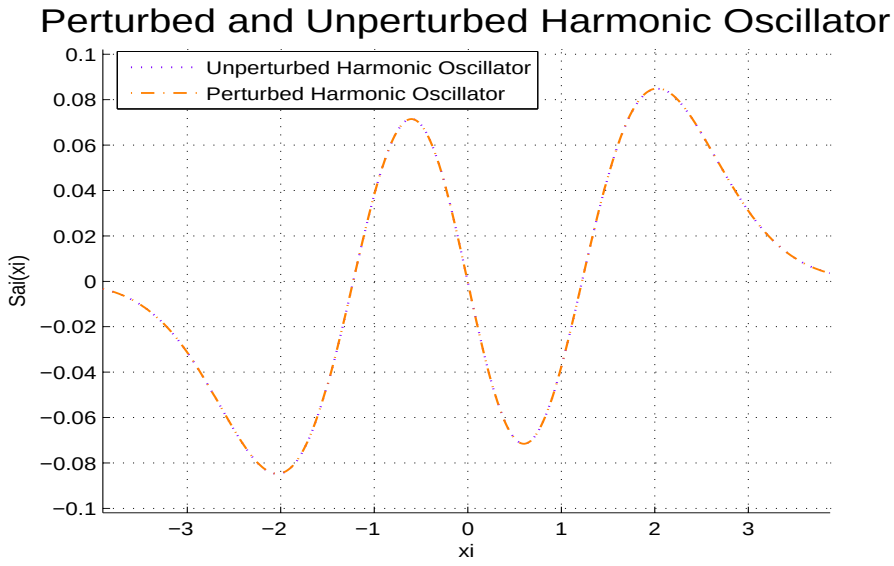

Figure 5.16: N_{dim}=16, $\eta = 100$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

The above Figures of (5.14), (5.15), and (5.16) illuminate the fact that by changing the matrix dimension for the same solution and with the same ‘‘strength’’ for the

perturbation, we obtain nearly the same graph.

Next, we examine the effect of changing η. Remember, smaller η, means larger β which means stronger perturbation ($\eta = 1/\beta$).

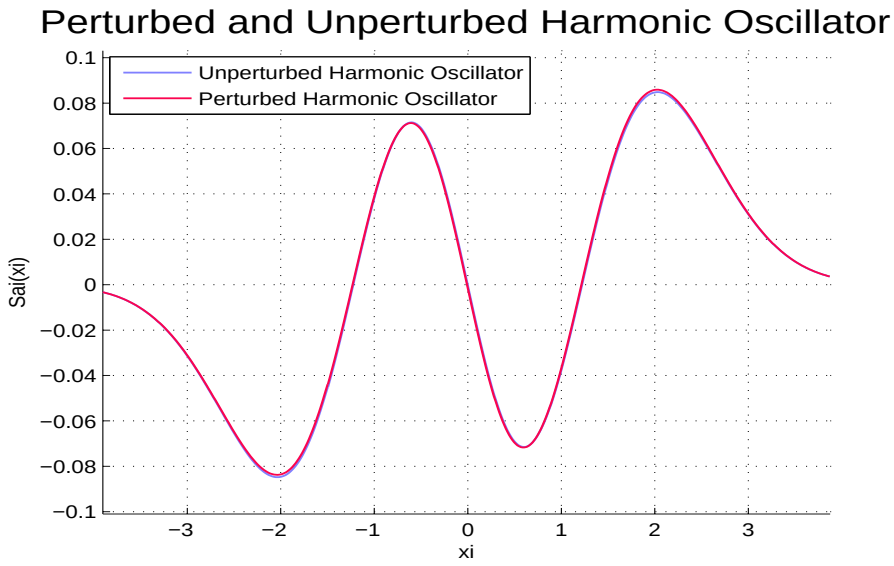

Figure 5.17: N_{dim}=5, $\eta = 10$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

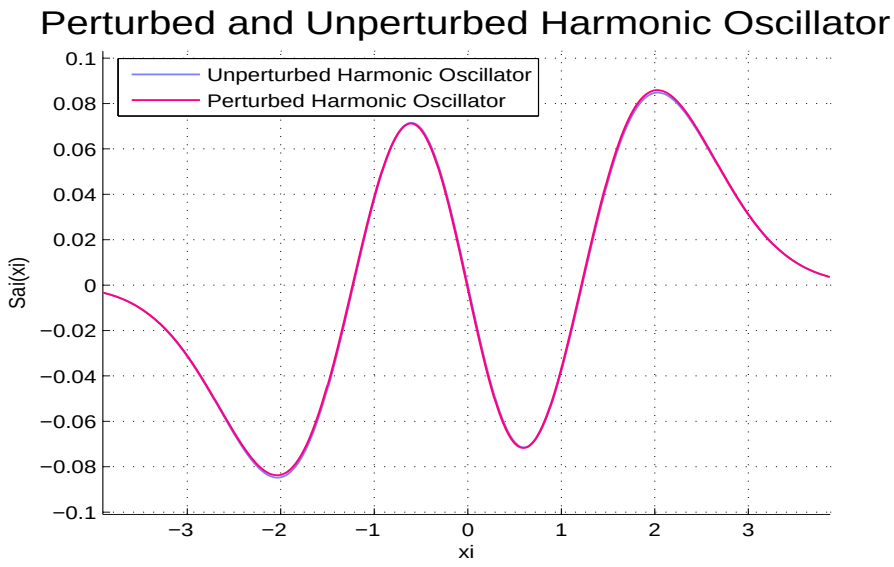

Figure 5.18: N_{dim}=10, $\eta = 10$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

From the plot (5.18) it is obvious that by changing the matrix dimension, for the same perturbation, we obtain results which are virtually indistinguishable. These results show the rapid convergence of the series expansions for expressing perturbed eigenfunctions in terms eigenfunctions of the harmonic oscillator.

As can be expected, by changing the perturbation strength, we should be able to recognize the change in the eigenfunctions of the perturbed harmonic oscillator. We can examine this perturbation for two matrix dimensions as follows. In Figure (5.19)

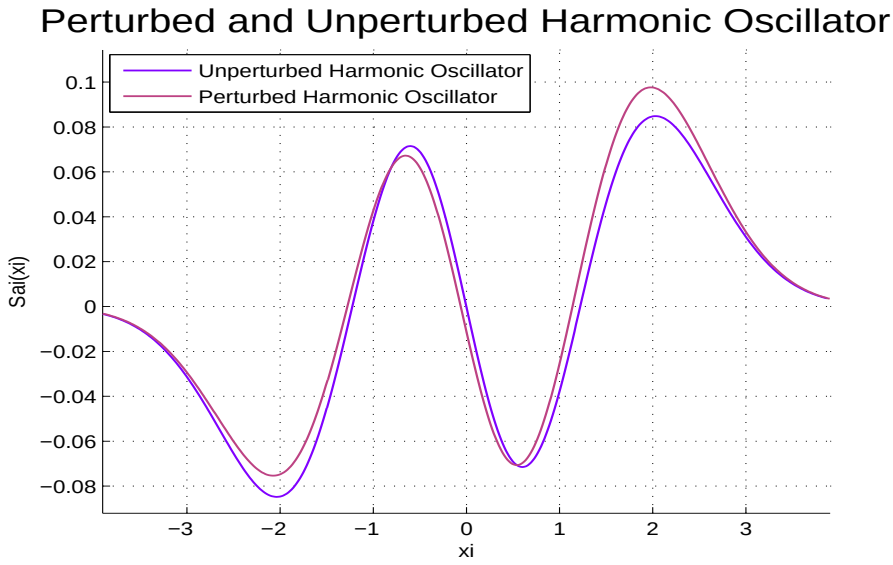

Figure 5.19: N_{dim}=8, $\eta = 1$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

and (5.20) with η being one, we have a comparatively strong perturbation.

As explained thoroughly before, in the case of $r = 2r' + 1$ no decoupling of the eigensystem matrix can take place. The only exception is when the diagonal terms is much stronger compared to the off-diagonal one. Now, we compare these two situations by examining A_{mn} and its eigenpairs for both cases.

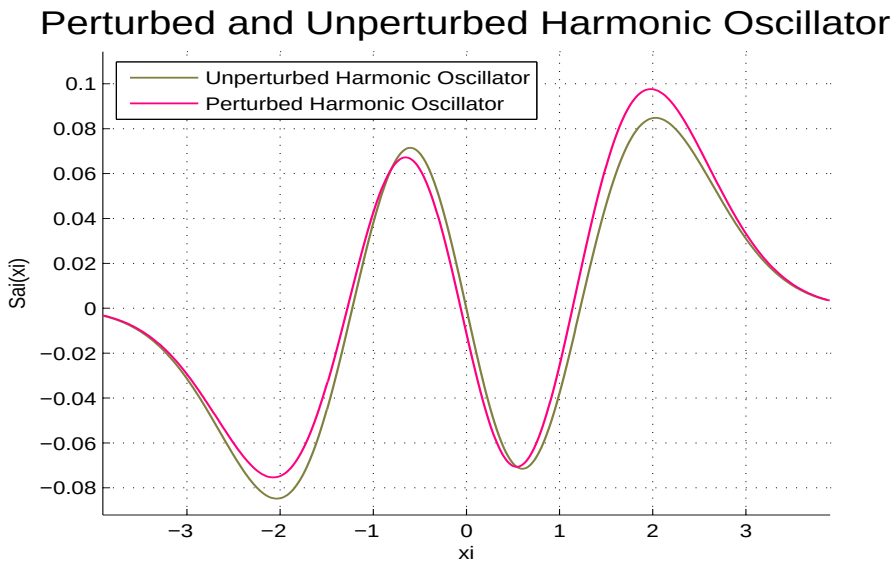

Figure 5.20: N_{dim}=5, $\eta = 1$, $r = 1$, 3rd eigensolution of Perturbed Harmonic Oscillator

A_{mn} for the non-decoupling case is:

$$A_{mn} = \begin{bmatrix} 0.5 & 0.5 & 0 & 0 & 0 & 0 \\ 0.5 & 1.5 & 0.25 & 0 & 0 & 0 \\ 0 & 0.25 & 2.5 & 0.0625 & 0 & 0 \\ 0 & 0 & 0.0625 & 3.5 & 0.0104 & 0 \\ 0 & 0 & 0 & 0.0104 & 4.5 & 0.0013 \\ 0 & 0 & 0 & 0 & 0.0013 & 5.5 \end{bmatrix}$$

Eigenvalues and the corresponding eigenvectors for $N_{dim} = 5$, $\eta = 1$ and $r = 1$ are as follows.

Eigenvalues:

$$\begin{bmatrix} 0.2887 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.6450 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.5623 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.5039 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.5001 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5.5000 \end{bmatrix}$$

the corresponding eigenvectors:

$$\begin{bmatrix} 0.9202 & -0.3865 & -0.0620 & -0.0014 & 0 & 0 \\ 0 & 0.9956 & 0 & 0.0933 & 0 & 0 \\ 0.0440 & 0.2594 & -0.9626 & -0.0642 & 0.0003 & 0 \\ -0.0009 & -0.0087 & 0.0642 & -0.9978 & 0.0104 & 0 \\ 0 & 0 & -0.0003 & 0.0104 & 0.9999 & 0.0013 \\ 0 & 0 & 0 & 0 & -0.0013 & 1 \end{bmatrix}$$

The following Figure (5.21) is a graph for the eigenvalues for $N_{dim} = 5$ with odd order perturbation. From the graph, it can be deduced that these eigenvalues are in ascending order which is the right order. The reason for having 6-by-6 matrix is that the eigenvalues and the corresponding eigenvectors start from 0^{th} solution to the fifth solution.

A_{mn} for matrix dimension ten is:

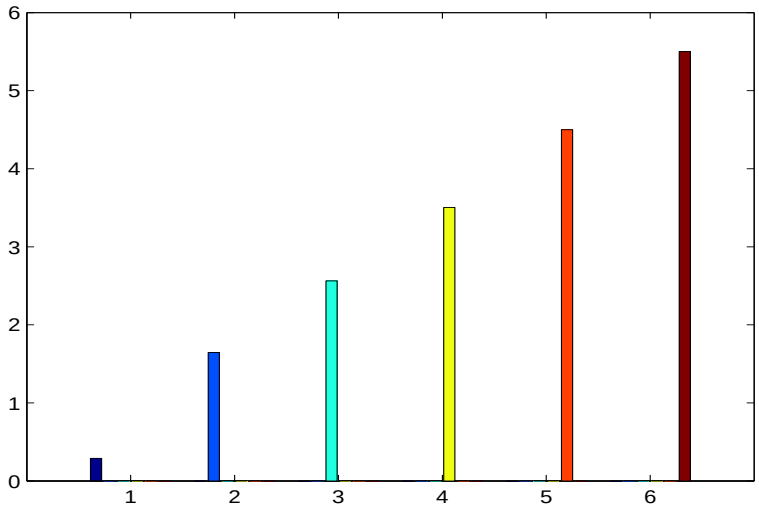

Figure 5.21: The graph of the Eigenvalues for N_{dim}=5, $r = 1$, $\eta = 1$

$$A_{mn} = \begin{bmatrix} 0.5 & 0.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 1.5 & 0.25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.25 & 2.5 & 0.0625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.5 & 0.0104 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0104 & 4.5 & 0.0013 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0013 & 5.5 & 0.0001 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0001 & 6.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10.5 \end{bmatrix}$$

The eigenvalues and the corresponding eigenvector for matrix dimension ten with the same η and r is

Eigenvalues:

$$\begin{bmatrix} 0.9661 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.8458 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4.5123 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6.5001 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2.2383 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3.5846 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5.5014 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7.5 \end{bmatrix}$$

The corresponding eigenvectors:

$$\begin{bmatrix}
-0.9202 & 0.3865 & 0.0620 & -0.0014 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.3889 & 0.8850 & 0.2557 & -0.0084 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.0440 & -0.2594 & 0.9626 & -0.0642 & 0.0003 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.0009 & 0.0087 & -0.0642 & -0.9978 & 0.0104 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.0104 & 0.9999 & -0.0013 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -0.0013 & -1 & 0.0001 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.0001 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}$$

Apparently, studying eigenvalues and eigenvectors for $N_{dim} = 10$ shows misplacement of the last two columns. This misplacement of columns happened after the appearance of some sort of symmetry in matrix A_{mn}.

Our eigenvalues are shifted to another column their corresponding eigenvectors are shifted to the corresponding columns.

The following graphs (5.23 - 5.26) show for different odd monomial perturbations with a fixed N_{dim}.

As expected by increasing the order of perturbation, the harmonic oscillator is perturbed correspondingly.

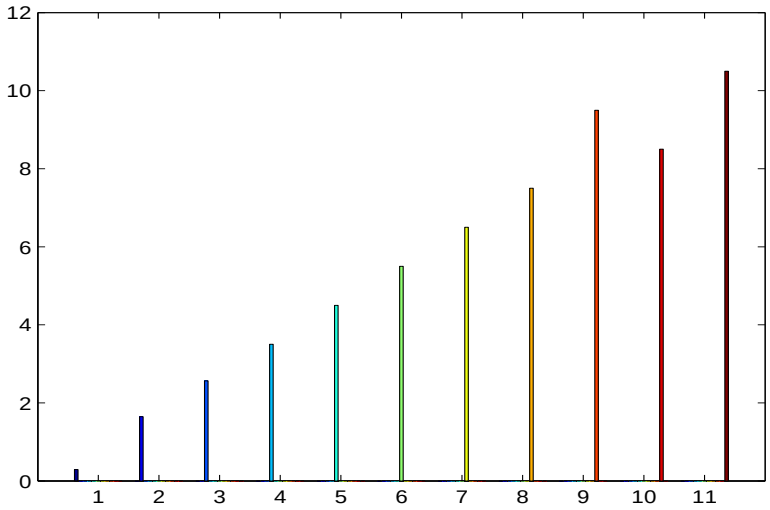

Figure 5.22: The graph of the Eigenvalues for N_{dim}=8, $r = 2$, $\eta = 1$

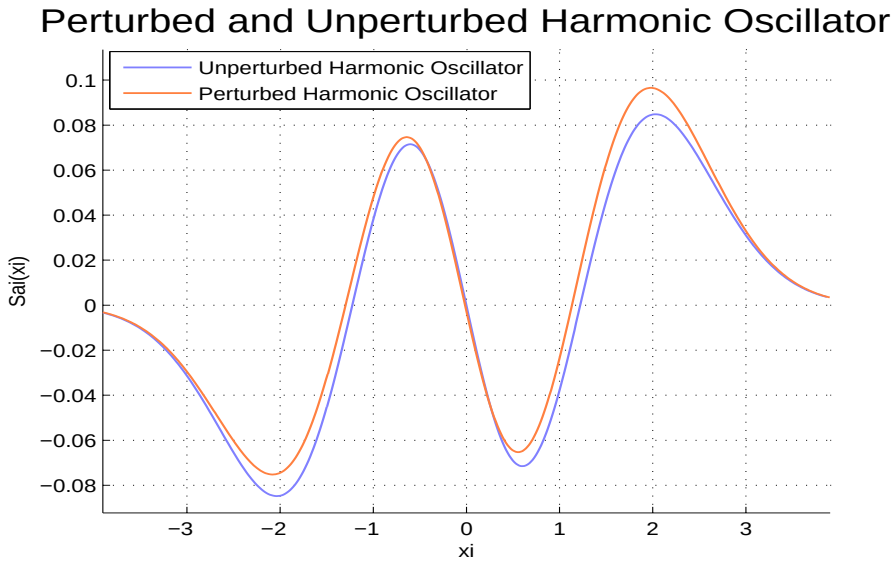

Figure 5.23: N_{dim}=9, $r = 3$, $\eta = 5$, 3[rd] eigensolution of Perturbed Harmonic Oscillator

5.2 Conclusion

Our numerical results show a strong indication for the validity of our theoretical considerations and their numerical implementation. These graphs show the robustness of the numerical technique for perturbation powers vanishing small to very large values.

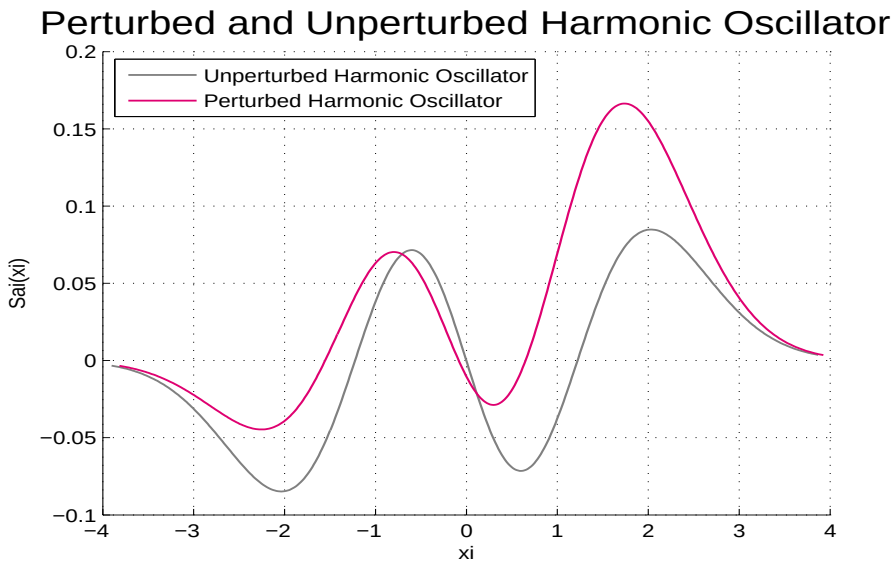

Figure 5.24: N_{dim}=9, $r = 5$, $\eta = 5$, 3rd eigensolution of Perturbed Harmonic Oscillator

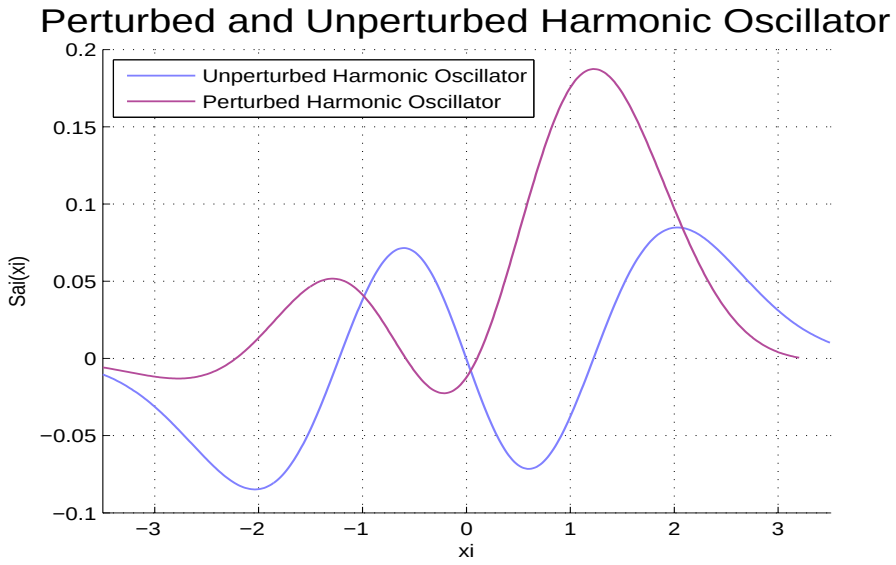

Figure 5.25: N_{dim}=9, $r = 7$, $\eta = 5$, 3rd eigensolution of Perturbed Harmonic Oscillator

In contrast to the perturbative and/or asymptotic approaches our proposed formulation tackles very weak to very strong perturbations in a unified form.

This is a very encouraging result and we feel satisfied that we could achieve all our objectives with one stroke.

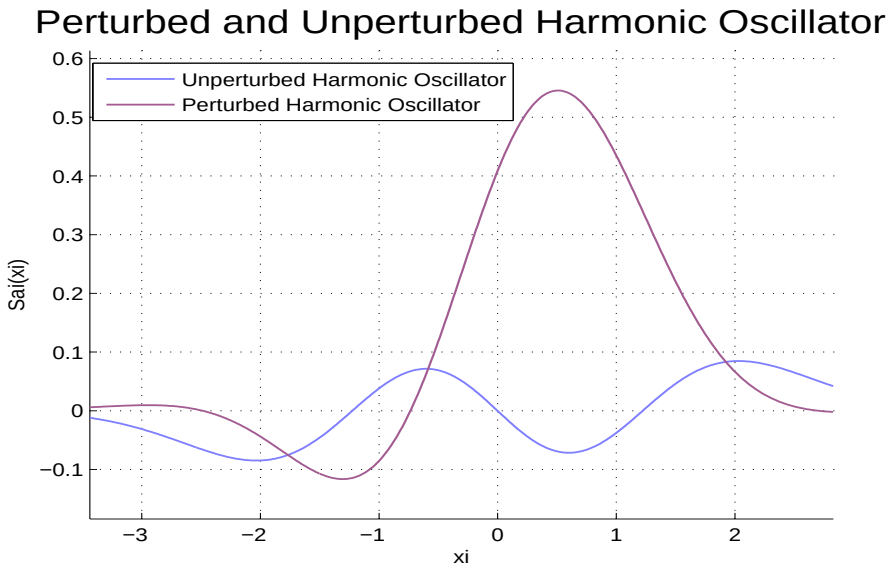

Figure 5.26: N_{dim}=9, $r = 9$, $\eta = 5$, 3rd eigensolution of Perturbed Harmonic Oscillator

Our result also testify the accuracy of the developed novel recurrence formula devised for the involved integrals and also for the representation of the Hermite polynomials.

Chapter 6

Future Work

6.1 Introduction

In the following sections, we will review a straight forward methodology for implementing polynomially perturbed 1D harmonic oscillator and linearly-perturbed harmonic oscillator in two dimensions. The involved steps follow the same logical explanation as described in Chapters 5 and 6. we have provided the lay out of our proposed methodology for possible future works pertaining to this research. This section gives a theoretical explanation on how problems related to the polynomially perturbed harmonic oscillators can be tackled.

6.2 Polynomially Perturbed Harmonic Oscillators

The results obtained in Chapter 4 can be utilized to solve polynomially perturbed harmonic oscillators. Our previous auxiliary problem can be exploited as a new auxiliary problem for our new ‘‘original’’ problem. The solutions of the ideal harmonic oscillator

$$-\frac{d^2}{d\xi^2}\psi(\xi)+\frac{1}{2}\xi^2\psi(\xi)=\widehat{E}\,\psi(\xi) \tag{6.1}$$

is known to us. Equation (6.1) is scaled version of the following equation:

$$-\frac{\hbar^2}{2m_0}\,\frac{d^2}{dx^2}\varphi(x)+\frac{1}{2}m_0\omega^2x^2\varphi(x)=E\,\varphi(x) \tag{6.2}$$

By utilizing the above auxiliary problem and based on our methodology, we aim at solving our new original problem, which is:

$$-\frac{\hbar^2}{2m_0}\,\frac{d^2}{dx^2}\widetilde{\varphi}(x)+\frac{1}{2}m_0\omega^2x^2\widetilde{\varphi}(x)+\sum_{r=0}^{R}\hbar\omega\sqrt{\Big(\frac{m_0\omega}{\hbar}\Big)^r}\,\beta_r x^r\widetilde{\varphi}(x)=\widetilde{E}\,\widetilde{\varphi}(x) \tag{6.3}$$

Replacing x by a dimensionless variable ξ ($x=\xi/\sqrt{\alpha}$) and using the equation (4.56) Chapter (4), the following relation results:

$$-\frac{\hbar^2}{2m_0}\alpha\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)+\frac{1}{2}m_0\omega^2\frac{1}{\alpha}\xi^2\widetilde{\psi}(\xi)+\sum_{r=0}^{R}\hbar\omega\sqrt{\Big(\frac{m_0\omega}{\hbar}\Big)^r}\,\beta_r\frac{1}{\sqrt{\alpha^r}}\xi^r\widetilde{\psi}(\xi)=\widetilde{E}\widetilde{\psi}(\xi) \tag{6.4}$$

Factorizing out the coefficient of the second term $(m_0\omega^2/\alpha)$, we have

$$\begin{aligned}\frac{m_0\omega^2}{\alpha}\Bigg[&-\frac{\hbar^2}{2m_0}\frac{\alpha}{m_0\omega^2}\alpha\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi)+\frac{1}{2}\xi^2\widetilde{\psi}(\xi)\\&+\sum_{r=0}^{R}\frac{\alpha}{m_0\omega^2}\hbar\omega\sqrt{\Big(\frac{m_0\omega}{\hbar}\Big)^r}\,\beta_r\frac{1}{\sqrt{\alpha^r}}\xi^r\widetilde{\psi}(\xi)\Bigg]=\widetilde{E}\widetilde{\psi}(\xi)\end{aligned} \tag{6.5}$$

Setting the coefficient of the first term to one, α can be obtained as:

$$\alpha = \frac{m_0\omega}{\hbar} \tag{6.6}$$

Therefore, equation (6.5) can be rewritten as:

$$\hbar\omega\left[-\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \frac{1}{2}\xi^2\widetilde{\psi}(\xi) + \sum_{r=0}^{R}\beta_r\xi^r\widetilde{\psi}(\xi)\right] = \widetilde{E}\widetilde{\psi}(\xi) \tag{6.7}$$

which can be represented in the following alternative form:

$$-\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \frac{1}{2}\xi^2\widetilde{\psi}(\xi) + \sum_{r=0}^{R}\beta_r\xi^r\widetilde{\psi}(\xi) = \widehat{\widetilde{E}}\widetilde{\psi}(\xi) \tag{6.8}$$

Writing equation (6.8) more explicitly we obtain:

$$-\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \frac{1}{2}\xi^2\widetilde{\psi}(\xi) + \left(\beta_0\xi^0 + \beta_1\xi^1 + \cdots + \beta_R\xi^R\right)\widetilde{\psi}(\xi) = \widehat{\widetilde{E}}\widetilde{\psi}(\xi) \tag{6.9}$$

Multiplying equation (6.9) by $\psi(\xi)$ and equation (6.1) by $\widetilde{\psi}(\xi)$ and subtracting the resulting equations we arrive at:

$$\left[-\psi(\xi)\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \widetilde{\psi}(\xi)\frac{d^2}{d\xi^2}\psi(\xi)\right] - \left(\beta_0\xi^0 + \beta_1\xi^1 + \cdots + \beta_R\xi^R\right)\psi(\xi)\widetilde{\psi}(\xi) = \left(\widehat{E} - \widehat{\widetilde{E}}\right)\psi(\xi)\widetilde{\psi}(\xi) \tag{6.10}$$

Integrating both sides of equation (6.10) from $-\infty$ to $+\infty$ leads to:

$$\int_{-\infty}^{+\infty} d\xi \left[-\psi(\xi)\frac{d^2}{d\xi^2}\widetilde{\psi}(\xi) + \widetilde{\psi}(\xi)\frac{d^2}{d\xi^2}\psi(\xi)\right] - \int_{-\infty}^{+\infty} d\xi \left(\beta_0\xi^0 + \beta_1\xi^1 + \cdots + \beta_R\xi^R\right)\psi(\xi)\widetilde{\psi}(\xi) = \left(\widehat{E} - \widehat{\widetilde{E}}\right)\int_{-\infty}^{+\infty} d\xi\psi(\xi)\widetilde{\psi}(\xi) \quad (6.11)$$

The first integral at the left-hand side vanishes, as shown in Chapter (4). Consequently, we obtain:

$$\int_{-\infty}^{+\infty} d\xi \left(\beta_0\xi^0 + \beta_1\xi^1 + \cdots + \beta_R\xi^R\right)\psi(\xi)\widetilde{\psi}(\xi) = \left(\widehat{\widetilde{E}} - \widehat{E}\right)\int_{-\infty}^{+\infty} d\xi\psi(\xi)\widetilde{\psi}(\xi) \quad (6.12)$$

Writing more explicitly, we obtain:

$$\int_{-\infty}^{+\infty} d\xi\beta_0\xi^0\psi(\xi)\widetilde{\psi}(\xi) + \int_{-\infty}^{+\infty} d\xi\beta_1\xi^1\psi(\xi)\widetilde{\psi}(\xi) + \cdots + \beta_R\int_{-\infty}^{+\infty} d\xi\xi^R\psi(\xi)\widetilde{\psi}(\xi) = \left(\widehat{\widetilde{E}} - \widehat{E}\right)\int_{-\infty}^{+\infty} d\xi\psi(\xi)\widetilde{\psi}(\xi) \quad (6.13)$$

In this case, each individual perturbation term can be calculated based of our technique discussed thoroughly in Chapter (4). Therefore, we obtain:

$$\sum_{n=0}^{\infty}\left[\beta_0\langle U_m\Big|\xi^0\Big|U_n\rangle + \beta_1\langle U_m\Big|\xi^1\Big|U_n\rangle + \cdots + \beta_R\langle U_m\Big|\xi^R\Big|U_n\rangle\right]\alpha_n = \left[\widehat{\widetilde{E}} - (m+1/2)\right]\sum_{n=0}^{\infty}\alpha_n\delta_{mn} \quad (6.14)$$

Introducing the notation $A_{mn}^{(r)} = \beta_r \langle U_m | \xi^r \big| U_n \rangle$ equation (6.14) can be written in the following compact form:

$$\sum_{n=0}^{\infty} \left[\beta_0 A_{mn}^0 + \beta_1 A_{mn}^1 + \cdots + \beta_R A_{mn}^R \right] \alpha_n = [\widehat{\widetilde{E}} - (m + 1/2)] \alpha_m \tag{6.15}$$

6.3 2D Linearly Perturbed Harmonic Oscillators

Our research in this work allows for solving linearly perturbed harmonic oscillator problems in two dimension.

The following partial differential equation in 2D is used as an auxiliary problem for linearly perturbed harmonic oscillator:

$$-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\varphi(x,y) - \frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial y^2}\varphi(x,y) + \frac{1}{2}k_1 x^2 \varphi(x,y) + \frac{1}{2}k_2 y^2 \varphi(x,y) = E\varphi(x,y) \tag{6.16}$$

Here, $\hbar$ is the reduced Planck's constant; m_0 is the mass of the electron and k specifies the magnitude of the quadratic potential functions. Since our problem is in two-dimensional domain, we have second derivatives with respect to both x and y for the kinetic energy associated with the motions in x- and y-directions. In addition, for the potential term in the Schrödinger equation, two terms appear, one for the x- and the second one for the y-depenence.

Assuming a variable seperation for $\varphi(x,y)$, i.e., can be variable separated and written in the following way:

$$\varphi(x,y) = \varphi_1(x)\varphi_2(y) \tag{6.17}$$

and substituting into (6.16), we obtain:

$$\begin{aligned} -\frac{\hbar^2}{2m_0}\varphi_2(y)\left(\frac{d^2}{dx^2}\varphi_1(x)\right) - \frac{\hbar^2}{2m_0}\varphi_1(x)\left(\frac{d^2}{dy^2}\varphi_2(y)\right) \\ + \frac{1}{2}k_1x^2\varphi_1(x)\varphi_2(y) + \frac{1}{2}k_2y^2\varphi_1(x)\varphi_2(y) = E\varphi_1(x)\varphi_2(y) \end{aligned} \tag{6.18}$$

We divide both sides of equation by $\varphi_1(x)\varphi_2(y)$:

$$-\frac{\hbar^2}{2m_0}\frac{1}{\varphi_1(x)}\frac{d^2}{dx^2}\varphi_1(x) - \frac{\hbar^2}{2m_0}\frac{1}{\varphi_2(y)}\frac{d^2}{dy^2}\varphi_2(y) + \frac{1}{2}k_1x^2 + \frac{1}{2}k_2y^2 = E \tag{6.19}$$

Regrouping of the terms results in:

$$-\frac{\hbar^2}{2m_0}\frac{1}{\varphi_1(x)}\frac{d^2}{dx^2}\varphi_1(x) + \frac{1}{2}k_1x^2 - \frac{\hbar^2}{2m_0}\frac{1}{\varphi_2(y)}\frac{d^2}{dy^2}\varphi_2(y) + \frac{1}{2}k_2y^2 = E \tag{6.20}$$

the x- and y-dependent equations decouple, yielding:

$$-\frac{\hbar^2}{2m_0}\frac{1}{\varphi_1(x)}\frac{d^2}{dx^2}\varphi_1(x) + \frac{1}{2}k_1x^2\varphi_1(x) = E_1\varphi_1(x) \tag{6.21a}$$

$$-\frac{\hbar^2}{2m_0}\frac{1}{\varphi_2(y)}\frac{d^2}{dy^2}\varphi_2(y) + \frac{1}{2}k_2y^2\varphi_2(y) = E_2\varphi_2(y) \tag{6.21b}$$

$$E_1 + E_2 = E \tag{6.21c}$$

Following the same procedure as in Chapter (4) and performing the variable substitutions

$$x = \frac{\xi}{\sqrt{\alpha_1}} \tag{6.22a}$$

$$y = \frac{\eta}{\sqrt{\alpha_2}} \tag{6.22b}$$

we obtain:

$$-\frac{1}{2}\frac{d^2}{dx^2}\psi_1(\xi) + \frac{1}{2}\xi^2\psi_1(\xi) = \widehat{E}_1\psi_1(\xi) \tag{6.23a}$$

$$-\frac{1}{2}\frac{d^2}{dy^2}\psi_2(\eta) + \frac{1}{2}\eta^2\psi_2(\eta) = \widehat{E}_2\psi_2(\eta) \tag{6.23b}$$

The solution to the first equation leads to the eigenvalues $\widehat{E}_1$ and the corresponding eigenfunctions $\psi_1(\xi)$ can give us the eigenvalue and the corresponding to the eigenfunction:

$$\widehat{E}_1 \Longleftrightarrow \psi_1(\xi) \tag{6.24}$$

Equivalently, the solution to the second equation leads to the eigenvalue $\widehat{E}_2$ and the corresponding eigenfunction $\psi_2(\eta)$:

$$\widehat{E}_2 \Longleftrightarrow \psi_2(\eta) \tag{6.25}$$

Therefore, we have:

$$\psi_1(\xi) = \frac{1}{\sqrt{\sqrt{\pi}m!2^m}} H_m(\xi) e^{-1/2\xi^2} \Longleftrightarrow \widehat{E}_1^m \tag{6.26a}$$

$$\psi_2(\eta) = \frac{1}{\sqrt{\sqrt{\pi}n!2^n}} H_n(\eta) e^{-1/2\eta^2} \Longleftrightarrow \widehat{E}_2^n \tag{6.26b}$$

$$\psi_{m,n}(\xi,\eta) = \frac{1}{\sqrt{\sqrt{\pi}m!2^m}} H_m(\xi) e^{-1/2\xi^2} \frac{1}{\sqrt{\sqrt{\pi}n!2^n}} H_n(\eta) e^{-1/2\eta^2} \Longleftrightarrow \widehat{E}_1^m + \widehat{E}_2^n \tag{6.26c}$$

The Schrödinger Equation for the linearly perturbed two-dimensional has the form:

$$-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\widetilde{\varphi}(x,y) - \frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial y^2}\widetilde{\varphi}(x,y) + \frac{1}{2}k_1 x^2 \widetilde{\varphi}(x,y) + \frac{1}{2}k_2 y^2 \widetilde{\varphi}(x,y) + U(x,y)\widetilde{\varphi}(x,y) = \widetilde{E}\widetilde{\varphi}(x,y) \tag{6.27}$$

Multiplying the auxiliary equation by $\widetilde{\psi}(x,y)$ and the perturbed equation by $\psi(x,y)$, and subtracting the resulting equations, we obtain:

$$-\frac{\hbar^2}{2m_0}\left[\varphi(x,y)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\widetilde{\varphi}(x,y) - \widetilde{\varphi}(x,y)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x,y)\right] - U(x,y)\varphi(x,y)\widetilde{\varphi}(x,y) = \left(E-\widetilde{E}\right)\varphi(x,y)\widetilde{\varphi}(x,y) \tag{6.28}$$

Integrating both sides of equation with respect to x and y from $-\infty$ to $+\infty$ we obtain:

$$-\frac{\hbar^2}{2m_0}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdy\left[\varphi(x,y)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\widetilde{\varphi}(x,y)-\widetilde{\varphi}(x,y)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x,y)\right]$$
$$-\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdyU(x,y)\varphi(x,y)\widetilde{\varphi}(x,y)=\left(E-\widetilde{E}\right)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdy\varphi(x,y)\widetilde{\varphi}(x,y) \tag{6.29}$$

Consider the first integral at the left-hand side of the equation (6.29):

$$\begin{aligned}
&-\frac{\hbar^2}{2m_0}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdy\varphi(x,y)\frac{\partial^2}{\partial x^2}\widetilde{\varphi}(x,y)\\
&=\int_{-\infty}^{+\infty}dy\int_{-\infty}^{+\infty}dx\varphi(x,y)\frac{\partial^2}{\partial x^2}\widetilde{\varphi}(x,y)\\
&=\int_{-\infty}^{+\infty}dy\left\{\varphi(x,y)\frac{\partial^2}{\partial x^2}\widetilde{\varphi}(x,y)\Big|_{-\infty}^{+\infty}-\int_{-\infty}^{+\infty}dx\frac{\partial}{\partial x}\varphi(x,y)\frac{\partial}{\partial x}\widetilde{\varphi}(x,y)\right\}\\
&=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdy\left\{\frac{\partial}{\partial x}\varphi(x,y)\right\}\left\{\frac{\partial}{\partial x}\widetilde{\varphi}(x,y)\right\}
\end{aligned} \tag{6.30}$$

Rewriting the second integral at the left-hand side, we realize that the contributions from $\varphi(\partial^2\widetilde{\varphi}/\partial x^2)-\widetilde{\varphi}(\partial^2\varphi/\partial x^2)$ cancel out. Similarly, the contribution from $\varphi(\partial^2\widetilde{\varphi}/\partial y^2)-\widetilde{\varphi}(\partial^2\varphi/\partial y^2)$ cancel out.

Therefore, it can be concluded that the first integral at the left-hand side of (6.29) vanishes.

Consequently, we obtain:

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdyU(x,y)\varphi(x,y)\widetilde{\varphi}(x,y)=\left(\widetilde{E}-E\right)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dxdy\varphi(x,y)\widetilde{\varphi}(x,y) \tag{6.31}$$

Utilizing the transformations $x = \xi/\sqrt{\alpha_1}$ and $y = \eta/\sqrt{\alpha_2}$ and introducing following relationships

$$U(x,y) = V(\xi,\eta) \tag{6.32a}$$

$$\varphi(x,y) = \psi(\xi,\eta) \tag{6.32b}$$

$$\widetilde{\varphi}(x,y) = \widetilde{\psi}(\xi,\eta) \tag{6.32c}$$

we can write:

$$\begin{aligned}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \frac{1}{\sqrt{\alpha_1}}d\xi\frac{1}{\sqrt{\alpha_2}}d\eta V(\xi,\eta)\psi(\xi,\eta)\widetilde{\psi}(\xi,\eta) \\ = \left(\widetilde{E}-E\right)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \frac{1}{\sqrt{\alpha_1}}d\xi\frac{1}{\sqrt{\alpha_2}}d\eta\psi(\xi,\eta)\widetilde{\psi}(\xi,\eta)\end{aligned} \tag{6.33}$$

Substituting,

$$\psi_{mn}(\xi,\eta) \Longrightarrow \psi_m^{(1)}(\xi)\psi_n^{(2)}(\eta) \tag{6.34}$$

and then the series expansion

$$\widetilde{\psi}(\xi,\eta) = \sum_{\bar{m}}\sum_{\bar{n}} \alpha_{\bar{m}\bar{n}}\psi_{\bar{m}}^{(1)}(\xi)\psi_{\bar{n}}^{(2)}(\eta) \tag{6.35}$$

For illustrating the details of calculations, we consider two simple, yet relevant cases:

Case 1: Assume $V(\xi,\eta) = V^{(1)}(\xi) + V^{(2)}(\eta)$, then the elements of the interaction matrix can be written as follows:

$$\begin{aligned} A_{m\bar{m}n\bar{n}} &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} d\xi d\eta \left[V^{(1)}(\xi)+V^{(2)}(\eta)\right] \psi_m^{(1)}(\xi)\psi_n^{(2)}(\eta)\psi_{\bar{m}}^{(1)}(\xi)\psi_{\bar{n}}^{(2)}(\eta) \\ &= \int_{-\infty}^{+\infty} d\xi V^{(1)}(\xi)\psi_m^{(1)}(\xi)\psi_{\bar{m}}^{(1)}(\xi)\int_{-\infty}^{+\infty} d\eta \psi_n^{(2)}(\eta)\psi_{\bar{n}}^{(2)}(\eta) \\ &+ \int_{-\infty}^{+\infty} d\xi \psi_m^{(1)}(\xi)\psi_{\bar{m}}^{(1)}(\xi)\int_{-\infty}^{+\infty} d\eta V^{(2)}(\eta)\psi_n^{(2)}(\eta)\psi_{\bar{n}}^{(2)}(\eta) \\ &= B_{m\bar{m}}\delta_{n\bar{n}} + \delta_{m\bar{m}}C_{n\bar{n}} \end{aligned} \tag{6.36}$$

Here, we have defined the matrix elements $B_{m\bar{m}}$ and $C_{n\bar{n}}$ in the obvious fashion.

By substituting the result from equation (6.36), (6.35), (6.34) and (6.32) into the equation (6.33) we arrive at:

$$\sum_{\bar{m}}\sum_{\bar{n}} \alpha_{\bar{m}\bar{n}} A_{m\bar{m}n\bar{n}} = \left(\widetilde{E} - E_{mn}\right)\sum_{\bar{m}}\sum_{\bar{n}} \delta_{m\bar{m}}\delta_{n\bar{n}} \tag{6.37}$$

Case 2: Assume $V(\xi,\eta) = V^{(1)}(\xi)V^{(2)}(\eta)$

$$\begin{aligned} A_{m\bar{m}n\bar{n}} &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} d\xi d\eta V^{(1)}(\xi)V^{(2)}(\eta)\psi_m^{(1)}(\xi)\psi_n^{(2)}(\eta)\psi_{\bar{m}}^{(1)}(\xi)\psi_{\bar{n}}^{(2)}(\eta) \\ &= B_{m\bar{m}}C_{n\bar{n}} \end{aligned} \tag{6.38}$$

For carrying out numerical calculation for monomially and polynomially perturbed 2D harmonic oscillator the following considerations seem relevant:

Let us assume:

$$\begin{aligned} U^{(1)}(x) &= \beta_r x^r \qquad x = \frac{1}{\alpha_1}\xi && \text{(6.39a)} \\ U^{(1)}(x) &= V^{(1)}(\xi) \\ U^{(1)}(x) &= \beta_r x^r \\ &= \beta_r {\alpha_1}^{-r/2} \xi^r \\ &= V^{(1)}(\xi) && \text{(6.39b)} \end{aligned}$$

In view of this analysis, we start the following ansatz:

$$\begin{aligned} U^{(1)}(x) &= \beta_r {\alpha_1}^{r/2} x^r && \text{(6.40a)} \\ U^{(1)}(x) &= V^{(1)}(\xi) \\ U^{(1)}(x) &= \beta_r \xi^r \\ &= \beta_r {\alpha_1}^{r/2} {\alpha_1}^{-r/2} \xi^r \\ &= \beta_r \xi^r \\ &= V^{(1)}(\xi) && \text{(6.40b)} \end{aligned}$$

Similarly,

$$U^{(2)}(y) = \beta_s {\alpha_2}^{s/2} y^s \tag{6.41a}$$

$$\begin{aligned} U^{(2)}(y) &= V^{(2)}(\eta) \\ U^{(2)}(y) &= \beta_s {\alpha_2}^{s/2} {\alpha_2}^{-s/2} \eta^s \\ &= \beta_s \eta^s \\ &= V^{(2)}(\eta) \end{aligned} \tag{6.41b}$$

Calculating the involved integrals by utilizing our results from 1D case enables the determination of eigenfunctions of 2D perturbed harmonic oscillator for weak or strong excitations.

6.4 Summary

By utilizing the method developed for the computation of monomial perturbations of the harmonic oscillator, we demonstrated that we can solve some related problems such as polynomially perturbed 1D harmonic oscillator and 2D linearly perturbed harmonic oscillator.

Chapter 7

Conclusion

7.1 Introduction

This chapter is the round off the preceding chapters and accounts the conclusion that we have achieved by performing our research on monomial and polynomial perturbed harmonic oscillators. The first section summarizes Chapters 4 and 5 which where our main chapters. In Section 7.3, a conclusion is drawn from the objective we set in Chapter 1 and discusses those areas in which our research has made contributions. We provide the scope of future works related to our current research in Section 7.4. Section 7.5 is a reflection on research methodology and the numerical results achieved.

7.2 Summary of Chapters

In Chapters 4 and 5 we have extensively discussed monomially perturbed harmonic oscillator in one dimension. Numerous cases were analyzed numerically. In Chapter 4, we provided explanation for monomially perturbed harmonic oscillator. Therefore, by changing the ‘‘strength’’ of the perturbation, changes in characteristic of the system

can be studied from the figures. In Chapter 5, we discussed perturbation of harmonic oscillator numerically. In that Chapter 4, we did not confine our proposed method to a particular power of perturbation. Therefore, we can observe changes in system characteristics for any type of polynomial perturbation, which is probably the main result of this research project.

7.3 Research Contribution

Our results demonstrate that we have successfully accomplished our goals that we set in Chapter 1. We provided an innovative approach for the robust calculation of perturbed eigenvalues and eigenvectors for monomial perturbation of the harmonic oscillator. Utilizing the results for the monomial perturbation, we demonstrated that we can solve much more complex problem such as polynomially perturbed harmonic oscillators. Controlling this additional potential reveals that by choosing an arbitrary potential, we can control the distribution of eigenstates to some degree and thus obtaining a desirable degree of localization. This achievement through our research is significant in the realm of the quantum harmonic oscillator and its wide ranging applications.

7.4 Suggestion for Possible Future Research

Through our research, we have developed the ground for a fascinating series of potential research studies. A probable research can be named as sinusoidal perturbation. A further idea could be summation of a polynomial and a sinusoidal function as an induced potential. The latter problem can be calculated by obtaining the solution for the

polynomial and sinusoidal perturbation. For polynomial perturbation we can observe the result for the negative potentials. A large number of attractive research problems can be formulated and solved for two- and three-dimensional perturbed harmonic oscillators.

7.5 Conclusion

We have successfully accomplished our research objective, i.e. we have proved and shown in greater details that problems related to 1D monomial harmonic oscillators can be solved using our proposed methodology. Results obtained by applying our method have been shown in the form of figures in Chapter 5. Furthermore, we have provided sufficient ground work necessary for tackling similar problem in a two-dimensional scenario and also polynomial perturbation of 1D harmonic oscillator. Our methodology is easy to use and eliminates the limitations of traditional computation techniques. Further ideas would include the development of robust and efficient numerical schemes for the construction of problem-specific basis functions for modelling molecular dynamic problems and more complex systems such as nano-wire transistors.

Appendix A

Hamiltonian

A.1 Hamiltonian's Eqautions

The classical equation of motion for a mass m_0 moving in one dimension,x, under a force $F = -kx$, is

$$m_0 \frac{d^2x}{dt^2} = -kx. \tag{A.1}$$

which we write in the form

$$\frac{d^2x}{dt^2} = -\frac{k}{m_0}x \tag{A.2}$$

Assume a harmonic time-dependence

$$x(t) = x_0 e^{-i\omega t} \tag{A.3}$$

with $x(0) = x_0$ we obtain

$$\frac{d^2}{dt^2}x = -\omega^2 x \tag{A.4}$$

a comparison with (A.2) suggest the equality

$$\omega^2 = \frac{k}{m_0} \tag{A.5}$$

or, equivalently,

$$\omega = \sqrt{k/m_0} \tag{A.6}$$

For a particle with the mass m_0 and linear velocity v and the linear momentum $p = m_0 v$ the kinetic energy T can be calculated in the following equivalent forms:

$$\begin{aligned} T &= \frac{m_0 v^2}{2} \\ &= \frac{m_0^2 v^2}{2m_0} \\ &= \frac{p^2}{2m_0} \end{aligned} \tag{A.7}$$

Assuming a conservative field the force F can be represented as the negative gradient of a potential function V, which in one dimension has the from:

$$-\frac{dV(x)}{dx} = F \tag{A.8}$$

Taking the integral with respect to x of the terms at both sides of this equation and the relationship $F = -kx$ we obtain the following explicit form for the potential function:

$$\begin{aligned} V(x) &= \frac{1}{2}\, k\, x^2 \\ &= \frac{1}{2}\, m_0\, \omega^2\, x^2 \end{aligned} \tag{A.9}$$

These equations are derivatives of Hamiltonian function

$$H = T + V \tag{A.10a}$$

$$= \frac{p^2}{2\, m_0} + \frac{1}{2} m_0\, \omega^2\, q^2 \tag{A.10b}$$

or, equivalently

$$H = \frac{p^2}{2\, m_0} + \frac{1}{2} k\, q^2 \tag{A.11}$$

in physicist's notation.

Another function of fundamental significance is the Lagrange function which is the difference between the kinetic and the potential energy:

$$L = \frac{p^2}{2\,m_0} - \frac{1}{2} m_0\,\omega^2\,q^2 \tag{A.12}$$

Denoting the generalized coordinate q and the velocity $\dot{q}$ ($q = x$, $\dot{q} = \dot{x}$) the differential of the Lagrangian can be written in the form:

$$dL = \frac{\partial L}{\partial q} dq + \frac{\partial L}{\partial \dot{q}} d\dot{q}. \tag{A.13}$$

Introducing p by the definition

$$p = \frac{\partial L}{\partial \dot{q}} \tag{A.14}$$

the Hamiltonian can be written as

$$H = p\dot{q} - L \tag{A.15}$$

Considering H to be a function of p and q, the differential of H, dH, is

$$dH = -\dot{p}dq + \dot{q}dp \tag{A.16}$$

It follows from (A.16)

$$\dot{q} = \frac{\partial H}{\partial p} \tag{A.17}$$

and

$$-\dot{p} = \frac{\partial H}{\partial q}. \tag{A.18}$$

For a system described by l generalized coordinates and l generalized momenta, the Poisson bracket $\{\cdots, \cdots\}$ is defined as

$$\{u, v\} = \sum_{i=1}^{l} (\frac{\partial u}{\partial q_i}\frac{\partial v}{\partial p_i} - \frac{\partial v}{\partial q_i}\frac{\partial u}{\partial p_i}) \tag{A.19}$$

Based on the Poisson brackets the following equations are immediate:

$$\dot{q} = \{q, H\} \tag{A.20}$$

and

$$\dot{p} = \{p, H\}. \tag{A.21}$$

Furthermore, the following important relationship between q and p is valid:

$$\{q, p\} = 1 \tag{A.22}$$

Next, for given mathematical objects u and v we define the commutator $[\cdots, \cdots]$ by

$$[u, v] = uv - vu, \tag{A.23}$$

when u and v represent functions, the commutator is obviously zero. In this case, the correspondence between Poisson brackets and commutators is determined by the rule

$$\{q, p\} \iff \frac{1}{i\hbar}[q, p] \tag{A.24}$$

$\hbar$ is Planck's constant and i is imaginary unit.

From equation (A.23) and (A.24), it can be inferred that q and p satisfy the commutation condition

$$qp - pq = i\hbar. \tag{A.25}$$

A.1.1 Energy Quanta

By using the relationship between p and q as given in equation (A.22), we obtain energy states of the harmonic oscillator with classical Hamiltonian given by (A.11). We write p and q, respectively, as $\hat{p}$ and $\hat{q}$, in order to explicitly show that they should be considered as operators. We proceed similarly for the relevant observables. As shown in this thesis, the energy values of the harmonic or anharmonic oscillators are given by the eigenvalues of the discretized energy matrices. These can be determined by introducing the annihilation operator $\hat{a}$ and the creation operator $\hat{a}^\dagger$ which are,

respectively, deduced from differential operators in equation (4.23) and (4.24)

$$\hat{a} = \sqrt{\frac{m_0\,\omega}{2\,\hbar}}\left(\hat{q} + i\,\frac{\hat{p}}{m_0\,\omega}\right) \tag{A.26}$$

and

$$\hat{a}^\dagger = \sqrt{\frac{m_0\,\omega}{2\,\hbar}}\left(\hat{q} - i\,\frac{\hat{p}}{m_0\,\omega}\right). \tag{A.27}$$

The operators $\hat{p}$ and $\hat{q}$ can be obtained by inverting the equations (A.26) and (A.27):

$$\hat{q} = \sqrt{\frac{\hbar}{2\,m_0\,\omega}}\left(\hat{a} + \hat{a}^\dagger\right) \tag{A.28}$$

and

$$\hat{p} = \frac{1}{i}\sqrt{\frac{\hbar\,m_0\,\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right). \tag{A.29}$$

In order to have real eigenvalues, both $\hat{p}$ and $\hat{q}$ should be Hamiltonian operators. The definition of the Hermitian conjugate matrix of A which is shown by $A^\dagger$ is:

$$A^\dagger_{ij} = A^*_{ji}. \tag{A.30}$$

A matrix A is Hermitian if $A^\dagger = A$, or in other word, $A_{ij} = A^*_{ji}$.

As it is apparent from the definition, $\hat{a}$ is the Hermitian conjugate of $\hat{a}^\dagger$.

Since $\hat{p}$ and $\hat{q}$ satisfy commutation relation

$$[\hat{q}, \hat{p}] = i\,\hbar \tag{A.31}$$

while $[\hat{q}, \hat{q}] = [\hat{p}, \hat{p}] = 0$, we conclude that,

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{A.32}$$

By replacing q and p with $\hat{q}$ and $\hat{p}$ in the Hamiltonian equation (A.11) and by using equations (A.28) and (A.29), we arrive at:

$$H = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \tag{A.33}$$

The eigenvalues of H can be obtained from the eigenvalues of

$$\hat{M} = \hat{a}^\dagger \hat{a}. \tag{A.34}$$

As shown in this thesis, the eigenvalues of $\hat{M}$ are non-negative integers, therefore, energy eigenstates are given by

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega; \qquad \{n = 1, 2, \cdots\} \tag{A.35}$$

In this thesis we made extensive use of the (A.35) and the fact that the corresponding eigenfunction constitute an orthogonal complete set of analyzing functions. We applied the fact to determine eigenfunctions of harmonic oscillators by perturbed by arbitrary monomials of even or odd order an arbitrary weak or strong perturbation.

Appendix B

Publication

- P. Peidaee, A. R. Baghai-Wadji, ‘‘On the Calculation of Linearly-Perturbed Harmonic Oscillators,’’ in Proceedings of ACES, Applied Computational Electromagnetic Society Conference, Verona, Italy, March 2007.

- P. Peidaee, A. R. Baghai-Wadji, ‘‘On the Calculation of Polynomially-Perturbed Harmonic Oscillators,’’ in Proceedings of PIERS, Progress in Electromagnetic Research Symposium, Beijing, China, March 2007.

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