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A Finite Element Method Framework for Solving Schrödinger Eigenvalue Problem in 2D

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Thesis Approval

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Declaration

I am a student of the AAUP university number 201712754. I confirm that I worked on this Master's thesis myself. And I declare that I have complied with all regulations, instructions, Arab American University standards of Academic codes of conduct. I also adhere to the Dean's Council regulations in withdrawing their confirmation of this degree in case of any violations.

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Dedication

I dedicate this thesis with a special feeling of gratitude to my parents,

To my husband Nimir Qozah who inspired me,

To my children Leen and Zaina,

To all members of my friends which suppoted me ,

To all of my family.

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Abstract

The Finite Element Method (FEM) is considered as well-known technique for solve partial differential equations numerically. It is also originally developed for solving problems occur in engineering and mathematical physics. Moreover, it is a numerical method for solving complex problems like structural analysis, heat transfer, fluid flow and complex systems. In Finite Element Method, we divide the domain in one direction into cells and use polynomials for approximating a function over a cell. Whereas, if the domain has two directions we divide it into intervals sub-domains and a given system discretization into smaller, simpler parts that are called elements and these are connected by Nodes and we choose the basis functions to provide an approximations of the unknown solution within an element. The Finite Element Method formulation of a boundary value problem finally leads in a system of algebraic equations. The simple equations that model these finite elements are then assembled into a larger system of equations that models the entire problem. The FEM then approximates a solution by minimizing an associated error function via the calculus of variations.The basis functions has three different kinds of elements which are linear , quadratic element and cubic element.

In this work, we use only a linear elements because it a quicker than others. We apply the finite element method with double well-potential using three different domains. at The end of the thesis, we give a numerical examples with different

domains.

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Introduction

The use of Finite Element Method (FEM) is inevitable within the analysis of complex structures and other systems in a matrix formulation[8].we think the origins of such a powerful and applicable method doesn't belong to a specific person or school of though but it came as a result for co-ordinating different scientific developments [1]. The finite element method is developed for the first time by A. Hernnikoff in 1941 [5] .In 1956, turner and topp introduced Finite Elements Method, they also reached to stiffness matrix by calculating the displacement between nodes or beam which form the strain of the two-dimensional domain and the first book of FEM was published in this year [5]. In (1965-1972) Zienkiewicz and Cheung presented Finite Element Method in a wider way which applied it on any field problem and this is what we called ”variational form” , this period called the golden age of FEM [6].
In (1972-1991) a huge development of the finite element method and its application took place while producing the first professional FEM p-version code [18]. In (1992-2017)Industrial applications of Finite Element Method and development of material modeling [**?**, 1, 11]
Finite Element method has many applications in many fields such as Electric and Magnetic Fields, Nuclear Engineering, Mechanic Design and Thermal Conduction [7, 14, 20]. Here we present some Finite Element method literature presented by researchers in the field. The first one [26] is about heat transfer by Thermal Conduction in which the authors studied about using DEM–FEM coupling method and they used FEM to reduce computational time in heat transfer. The second one In [7] is about Electromagnetic in which the authors studied about Electromagnetic field effects on biological materials and they used FEM to solve The coupled

equations of electromagnetic wave propagation and heat transfer under LTNE assumption. In the third study, [7] is about Thermal Conduction too in which the authors studied about heat transfer by Thermal Analysis of cast-resin dry-type transformers and they used FEM to model temperature distribution of cast-resin transformers.

The Schrödinger equation is one of the equations which is studied in the field of a linear partial differential equations [24]. The Schrödinger equation is used for describing the wave function and understanding many quantum natural phenomena. The Schrödinger equation might be difficult to be solved in the theoretical and numerical method, some of these Separation Variable and WKB Approximation. we consider the eigenvalue problem of the time independent Schrodinger equation with a potential $\Psi(x)$ is solved based on the following form

$$Hu := -\Delta u + \psi u = Eu, \text{in } \Omega \tag{0.1}$$

$$u(x) = 0, x \in \partial\Omega \subseteq R^d \tag{0.2}$$

where $\Omega \subseteq \mathbb{R}$ is adomain with $\partial\Omega$ that is boundaries. $\Omega : R^d \to R$ is defined as a real valued potential. Meanwhile, on the left hand side

$$H = -\Delta + \psi$$

is defined as The Hamiltonian operator that correlates usually to the total energy. E and u are the corresponding eigenvalues and eigenfunctions of the problem, respectively it is referred to as quantum potential energy, the quantum potential is a term within the Schrödinger equation which describes the movement of quantum particles. By using variational form for the eigenvalue problem (1.1) we can find the eigenvalue λ and its associated eigenfunction$u(x) \in$

$W := H_0^1(\Omega)$ such that

$$a(u,v) = \int_\Omega (\nabla u(x).\nabla v(x) + \Psi(x)u(x)v(x))dx = \lambda \int_\Omega u(x)v(x)dx = \lambda(u,v) \qquad (0.3)$$

for all $v \in W$ by using Finite Element Method, we obtained the discretized problem of the eigenvalue problem (1.3) we can find the eigenvalues λ_h and associated eigenfunctions $u_h(x) \in V_h \subseteq W$ such that

$$a(u_h, v_h) = \lambda(u_h, v_h), \text{for all } v_h \in V_h \qquad (0.4)$$

conforming finite element space spanned by N_h nodal basis functions on some regular finite element mesh T_h with mesh size h. After the FEM discretization, one could apply eigenvalue algorithms, including QR-algorithm, to the N_h -dimensional finite element matrices to obtain the eigen-pairs (λ_h, u_h) [23].

In this thesis, we use the Finite Element method to solve in numerically the Schrödinger equation in two dimensions. In particular, we specifically solve Schrödinger equation along with the double well positional. the motivation behind this is the complexity to find an analytical solution for this partial differential equation while using the double well potential as the main potential in the equation. The Finite Element Method forms a very straightforward and simple way to solve this equation since it uses only linear elements to get the first few eigenvalues and eigenfunctions. We formulate the finite element method and also implement it using several numerical examples on two dimensional domains with different levels of complexity. the relative error values and produced results validate the approach.

The thesis shows in the first chapter the cases of the Schrödinger equation which include the particle in one a dimensional box, the particle with the constant potential and the Schrödinger equation of harmonic oscillator, we present also the derivation of Schrödinger's time independent equation. In the second chapter we shows the basics of basis functions and the double well potential to compute eigenvalues and eigenfunctions of Schrödinger equation with using FEM, which is a numerical method for solving partial differential equations in two or three space variables and used method for solving problems of engineering and mathematical models. In the third chapter, we apply the Finite Element method with different domain in Matlab program to obtain the eigenvalues and the eigenfunctions .

Chapter One

Schrödinger Equation and Potentials

In this chapter, we present some basic concepts of a Hamiltonians Mechanics and Schrödinger Equation.

1.1 Schrödinger Equation

The Schrödinger equation is considered an important development in the literature of quantum mechanics [15]. The Schrödinger equation using for describe the wavefunction and understand many quantum natural phenomena. there are two types of the Schrödinger Equation the first Schrödinger's time independent equation and the second Schrödinger's time dependent equation . Where Schrödinger equation :

$$Eu_{(x,t)} = -\frac{\hbar^2\nabla^2}{2m}u_{(x,t)} + \psi_{(x)}u_{(x,t)}$$

Where

- $\hbar$: is the Planck's constant divided by 2π:$1.05459 \times 10^3 2$ Joul*second .
- $u_{(x,t)}$: is the space and time defined wave function.
- m: is the mass of the particle.

- ∇^2: is the Laplacian Operator : $\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{dx^2}$.

- $\psi_{(x,t)}$: is the potential energy influencing the particle [8].

1.2 Background

Quantum theory tells us that Both of the light and material contain very small molecules when these molecules become small enough, they change into waves and these waves have similar characteristic light and matter consists of tiny particles which have wavelike properties associated with them. Light is composed of particles called photons and the light behaves like a wave, and matter is composed of atoms and atoms made electrons, protons, neutrons. It's only when the mass of a particle gets small enough that its wavelike properties show up. when we make the light brighter more electrons are emitted but all have the same kinetic energy . light comes in discrete packages, called photons, and each photon must have enough energy to eject a single electron. Otherwise, nothing happens. So, the energy of a single photon is:

$$E_{photon} = hf = h\omega \tag{1.1}$$

Where h is the Planck's constant and ω is the frequency of the photon (angular frequency. The relationship between momentum p and wavelength λ for matter waves is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} \tag{1.2}$$

and the relationship energy and frequency is

$$E = hf \tag{1.3}$$

The wavelength is called the de Broglie wavelength, and the relations

$$\lambda = \frac{h}{p},\ f = \frac{E}{h} \tag{1.4}$$

are called the de Broglie relations. There are the same relations between Energy E and wavelength λ for the particle

$$E = \frac{1}{2}m\nu^2 = \frac{p^2}{2m} \tag{1.5}$$

so,

$$E = \frac{h^2}{\lambda^2 2m} \tag{1.6}$$

Then

$$\lambda = \frac{h}{\sqrt{2mE}} \tag{1.7}$$

The relationship between λ and E is different for particles than for photons. The wave function is given by the formulation of wave-function

$$u_{(x,t)} = Ae^{i(kx-wt)} \tag{1.8}$$

where x position vector, t is the time, A is amplitude, k is a wave frequency and its equal $\frac{2\pi}{\lambda}$ and w angular frequency and its equal $2\frac{\pi}{T}$ where T is a period time.

1.3 Hamiltonian Mechanics

Hamiltonian mechanics is a mathematically advanced formulation of classical mechanics. it corresponds to the total energy where it's the sum of kinetic and potential energy traditionally denoted E and H.Historically, Hamiltonian mechanics was first by William Rowan Hamilton in 1833, starting from Lagrangian mechanics, a previous reformulation of classical mechanics introduced by Joseph Louis Lagrange in 1788. Like Lagrangian mechanics, Hamiltonian mechanics is equivalent to Newton's laws of motion in the framework of classical mechanics.

$$E = H \tag{1.9}$$

$$\hat{E}u = \hat{H}u \tag{1.10}$$

$$H = KineticEnergy + PotentialEnergy$$

$$H = \frac{1}{2}m\nu^2 + \frac{1}{2}Kx^2 \tag{1.11}$$

Where m is the mass of the particle , v is the velocity ,K is the spring force constant ,x is the string stretch length in m .

$$P = m\nu \rightarrow \nu = \frac{P}{m} \tag{1.12}$$

Where P is the momentum .

$$\hat{P} = \hat{P}_x = -i\hbar\frac{d}{d_x} \tag{1.13}$$

$$\hat{P}_x = -i\hbar\nabla \tag{1.14}$$

where ∇ is the gradient operator and it's equal $(\frac{\partial}{\partial_x}, \frac{\partial}{\partial_y}, \frac{\partial}{\partial_z})$, $\hbar$ is the reduced Planck constant and i is the imaginary unit.

$$\hat{E} = i\hbar\frac{d}{d_t} \tag{1.15}$$

$$k = \frac{1}{2}m\nu^2 = \frac{1}{2}P\nu = \frac{1}{2m}P^2 \tag{1.16}$$

$$\hat{k} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} = -\frac{\hbar^2}{2m}\nabla^2 \tag{1.17}$$

substituting equation 1.15 and equation 1.17 in equation 1.11, we have the Schrödinger equation:

$$i\hbar\frac{d}{dt}u_{(x,t)} = -\frac{\hbar^2}{2m}\nabla^2 u_{(x,t)} + \psi u_{(x,t)} \tag{1.18}$$

1.4 Derivation Schrödinger equation

The Schrödinger equation has two forms the time-dependent Schrödinger equation and the time-independent Schrödinger equation.

1.4.1 Schrödinger's time independent equation

The Schrödinger's time independent equation means that the quantum state of the electron does not change, and therefore the electron have a constant wave. we can find the electron density (i.e. the sizes and shapes of atomic and molecular orbits) using the wave function. We can solved the second order differential equations as Schrödinger Equation, by separation of variables. These separated solutions can then be used to solve the problem in general. We can derivation the Schrödinger's time independent equation by separation of variable : Assume that we can factorize between time $T(t)$ and space $v(x)$

$$u(x,t) = v(x)T(t) \tag{1.19}$$

Substitute equation 1.19 in Schrödinger equation 1.18, we have:

$$[-\frac{\hbar^2}{2m}\frac{d^2v(x)}{dx^2} + \psi(x)v(x)]T(t) = i\hbar v(x)\frac{dT(t)}{dt} \tag{1.20}$$

Put every thing that depends on x on the left and everything that depends on t on the right:

$$\frac{\frac{-\hbar^2}{2m}\frac{d^2v(x)}{dx^2} + \psi(x)v(x)}{v(x)} = \frac{i\hbar\frac{dT(t)}{dt}}{T(t)}, \text{where } T(t) \neq 0 \tag{1.21}$$

The right hand side is constant, let

$$\frac{i\hbar\frac{dT(t)}{dt}}{T(t)} = E \quad (1.22)$$

$$i\hbar\frac{dT(t)}{dt} = E\,T(t) \quad (1.23)$$

$$\frac{dT(t)}{dt} + \frac{iE}{\hbar}T(t) = 0 \quad (1.24)$$

$$T(t) = e^{\int \frac{-iE}{\hbar}}dt = C\,e^{\frac{-iEt}{\hbar}} \quad (1.25)$$

$$\frac{-\hbar^2}{2m}\frac{d^2v(x)}{dx^2} + \psi(x)v(x) = E\,v(x) \quad (1.26)$$

This equation is called Time independent Schrödinger equation.

$$u(x,t) = v(x)T(t) = v(x)e^{\frac{-iEt}{\hbar}} \quad (1.27)$$

We can solve this equation when determine the potential .

1.4.2 Schrödinger Equation with a constant potential

Assume $\psi(x) = \psi_0$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + \psi_0 u(x) = E\,u(x) \quad (1.28)$$

$$\frac{d^2u(x)}{dx^2} = \frac{2m}{\hbar^2}(\psi_0 - E)u(x) \quad (1.29)$$

Let $K^2 = \frac{2m}{\hbar^2}(\psi_0 - E)$

For $E > \psi_0$, there are two solution of the wave function :

$$e^{iKx}\,,\,e^{-iKx}$$

Where $K = \frac{\sqrt{2m\psi_0 - E)}}{\hbar}$, these are two waves traveling in opposite directions with the same energy (and magnitude of momentum), we could also use the linear combinations of the two solutions

$$sin(Kx) \text{ and } cos(Kx)$$

For $E < \psi_0$, the solutions are also correct but K becomes imaginary

$$K = ik = \frac{\sqrt{2m(E-\psi_0)}}{\hbar}$$

The solutions are

$$e^{Kx}, e^{-Kx}$$

These are not waves at all, but real exponentials. Note that these are solutions for regions where the particle is not allowed classically, due to energy conservation; the total energy is less than the potential energy. In the case of free particle that means $\psi = 0$, the Schrödinger equation became :

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = Eu(x) \tag{1.30}$$

$$\frac{d^2u(x)}{dx^2} = -\frac{2m}{\hbar^2}Eu(x) \tag{1.31}$$

$$\frac{d^2u(x)}{dx^2} = -K^2u(x), \text{where } K = \frac{\sqrt{2mE}}{\hbar} \tag{1.32}$$

$$\frac{d^2u(x)}{dx^2} + K^2u(x) = 0 \tag{1.33}$$

the solution of equation 1.33 is

$$u(x) = Ae^{-iKx} + Be^{iKx} \tag{1.34}$$

1.4.3 The Particle in a One Dimensional Box

The particle in a box is a very simple to understand the behavior of a particle , we need to specify the potential for H

$$\Psi(x) = \begin{cases} 0 : 0 < x < L \\ \infty : otherwise \end{cases} \tag{1.35}$$

Where L is a length

$$Hu = Eu \tag{1.36}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + \psi_0 u(x) = Eu(x) \tag{1.37}$$

We have $\Psi = 0$ inside the box. Thus, the time-independent Schrödinger Equation can be reduced to

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} = Eu(x) \tag{1.38}$$

$$\frac{d^2u(x)}{dx^2} = -\frac{2m}{\hbar^2}Eu(x) \tag{1.39}$$

$$\frac{d^2u(x)}{dx^2} = -K^2u(x) \tag{1.40}$$

Where $K = \frac{\sqrt{2mE}}{\hbar}$ is a constant independently x, when $u(x) = e^{rx}$

$$\frac{du(x)}{dx} = re^{rx}$$
$$\frac{d^2u(x)}{dx^2} = r^2e^{rx}$$

substitute in equation 1.40, we have:

$$r^2e^{rx} = -K^2e^{rx}$$

Dividing e^{rx}, we have :

$$r^2 = -K^2 \tag{1.41}$$

Then

$$r = iK,\ r = -iK \tag{1.42}$$

If r_1, r_2 complex $\alpha \mp \beta i$:

$$u(x) = e^{\alpha} c_1 \cos(\beta x) + c_2 \sin(\beta x), \text{where } c_1, c_2 \text{ are constants}$$

$$u(x) = c_1 \cos(Kx) + c_2 \sin(Kx)$$

Equivalent to :

$$u(x) = Ae^{-iKx} + Be^{iKx} \tag{1.43}$$

or

$$u(x) = A\cos(Kx) + B\sin(Kx) \tag{1.44}$$

$$u(x,t) = Ae^{-iKx}e^{\frac{-iEt}{\hbar}} + Be^{iKx}e^{\frac{-iEt}{\hbar}} \tag{1.45}$$

where $e^{\frac{-iEt}{\hbar}}$ function of time, substitute Boundary conditions in equation 1.45

$$u(x \leqslant 0) = 0$$

$$u(x \geqslant L) = 0$$

$$u(0) = A\cos(0x) + B\sin(0x) = A$$

$$u(L) = Bsin(KL) = 0$$

$$sin(Kl) = 0 \text{ ,so}$$

$$kL = n\pi$$

$$k_n = \frac{n\pi}{L}, n \in \mathbb{Z}$$

$$u_n(x) = B\sin\left(\frac{n\pi x}{L}\right), n = 1, 2, 3, ...$$

$$K_n = \frac{\sqrt{2mE_n}}{\hbar} = \frac{n\pi x}{L}$$

$$2mE_n = \frac{n^2\pi^2\hbar^2}{L^2}$$

Then we have

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Where n is a quantum number .

$$u_n(x) = B\sin\left(\frac{n\pi}{L}x\right) \tag{1.46}$$

The square of the wave function (u^2) gives the probability of finding the electron anywhere in space, the probability of finding the particle-wave inside the box is unity (it is 1).this is the normalizing requirement

$$\int_{-\infty}^{\infty} u(x)u^*(x)dx = 1 \tag{1.47}$$

To find the value of B we solve the normalizing requirement

$$B^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right)dx = 1$$

Let $y = \frac{n\pi x}{L}$ then we have $x = \frac{Ly}{n\pi}$ and $dx = \frac{L}{n\pi}dy$, substitute y in the previous expression

$$\frac{LB^2}{n\pi}\int_0^{n\pi} sin^2(y)dy$$
$$\frac{LB^2}{n\pi}\int_0^{n\pi} \frac{1-cos(2y)}{2}dy$$
$$\frac{LB^2}{n\pi}\left[\frac{y}{2} - \frac{sin2y}{4}\Big|_0^{n\pi}\right]$$
$$\frac{LB^2}{n\pi}\left[\frac{n\pi}{2}\right] = \frac{LB^2}{2}$$
$$\frac{LB^2}{2} = 1$$
$$B = \sqrt{\frac{2}{L}}$$

Now, we can substitute the value of B into equation 1.47, we have:

$$u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \tag{1.48}$$

If the potential inside the well $\Psi(x) = P$, we solve again the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + Pu(x) = Eu(x) \tag{1.49}$$

Rearranging equation:

$$\frac{d^2u(x)}{dx^2} = -\frac{2m(E-P)u(x)}{\hbar^2} \tag{1.50}$$

For the regions outside the well, the particle may have energy that is greater than or less than the potential energy of the well. For $E > P$, the particle is said to be in a free state and we find $K = \frac{\sqrt{2m(E-P)}}{\hbar}$. For $E < P$, the particle is said to be in a bound state and we define $\alpha = \frac{\sqrt{2m(E-P)}}{\hbar}$.

We have a second order differential equation where the second derivative of the wave function $u(x)$ is equal the positive of the wave function times some constants. Trigonometric functions do not satisfy this condition, but exponentials do. Thus, we have

$$u = Ce^{-i\alpha x} + De^{i\alpha x} \tag{1.51}$$

The function takes on a trigonometric form. In the region where $x < 0$, we see that as $x \to -\infty$ the coefficient $C \to \infty$. Since, the wave function must have a finite total integral, the term C must be negated ; so we have

$$u = De^{i\alpha x}, \text{ where } x < 0 \tag{1.52}$$

By the same condition, we see that for the region where $x > L$, as $x \to \infty$, then $D \to \infty$ this term must be negated. Thus, we have

$$u = Ce^{-i\alpha x}, \text{ where } x > L \tag{1.53}$$

1.5 Solution of Schrodinger's equation for harmonic oscillator

In classical mechanics, a harmonic oscillator of mass m and spring constant k is described by Hooke's law and the equation of motion is

$$F = -kx = ma, \text{where } a = \frac{d^2x}{dt^2} \tag{1.54}$$

where k is a spring constant, x is a displacement and m is a mass.

$$-kx = m\frac{d^2x}{dt^2} \tag{1.55}$$

we have

$$x = Ae^{i\sqrt{\frac{k}{m}}t} + Be^{-i\sqrt{\frac{k}{m}}t} \tag{1.56}$$

The potential energy of a Harmonic Oscillator is

$$\Psi(x) = \tfrac{1}{2}kx^2 = \tfrac{1}{2}m\omega^2x^2$$

where ω is an angular frequency and it is equal $\sqrt{\frac{k}{m}}$. The time-independent Schrödinger equation for Simple Harmonic Oscillator(SHO) is

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \frac{1}{2}m\omega^2x^2u = Eu \tag{1.57}$$

We have a singular point at $\mp\infty$ because of x^2 in the potential of the equation . In order to solve this differential equation, we need to get its equivalent standard form, let $\xi = \alpha\, x$ where ξ is a unit free and $[\alpha]$ is a length

$\frac{d}{dx} = a\frac{d}{d\xi}$ and $\frac{d^2}{dx^2} = \alpha^2\frac{d^2}{d\xi^2}$ substitute it in equation 1.58, we have

$$-\frac{\hbar^2\alpha^2}{2m}\frac{d^2u}{d\xi^2} + \frac{1}{2}m\omega^2\alpha^2\xi^2u = Eu \tag{1.58}$$

Rearrange the time-independent Schrödinger equation for SHO :

$$\frac{d^2u}{d\xi^2} + \frac{2mE}{\hbar^2\alpha^2}u(\omega) - \frac{m^2\omega^2}{\hbar^2\alpha^2}\xi^2\omega^2 u(\omega) = 0 \tag{1.59}$$

where $\frac{m^2\omega^2\alpha^2}{\hbar^2} = 1$ then $\alpha^2 = \frac{\hbar}{m\omega}$ therefore, $\xi = \frac{x}{\alpha} = \frac{x}{\sqrt{\frac{\hbar}{m\omega}}} = \sqrt{\frac{m\omega}{\hbar}}x$

The Simple Harmonic Oscillator Schrödinger equation can be written in terms of dimensionless variable by making the coefficient of ξ^2 unity and introducing a dimensionless number ϵ, let $\epsilon = \frac{2mE}{\hbar^2\alpha^2}$

the Schrödinger equation became :

$$\frac{d^2u}{d\xi^2} = (\xi^2 - \epsilon)u \tag{1.60}$$

as $\epsilon \to \mp\infty$, ξ^2 became largest than ϵ because ϵ is a constant then :

$$\frac{d^2u}{d\xi^2} \cong \xi^2 u \tag{1.61}$$

The wave-equation is :

$$u = \xi^k e^{\alpha}\frac{\xi^2}{2} \tag{1.62}$$

Let $\alpha = \mp 1$ the equation became :

$$u = A\xi^k e^{\frac{-\xi^2}{2}} + B\xi^k e^{\frac{\xi^2}{2}}, \text{as}\xi \to \mp\infty \tag{1.63}$$

Without loss of generality the equation became :

$$v = h(\xi)e^{\frac{-\xi^2}{2}} \tag{1.64}$$

Derive the general solution :

$$\frac{du}{d\xi} = \frac{dh}{d\xi}e^{\frac{-\xi^2}{2}} - \xi u \tag{1.65}$$

$$\frac{d^2u}{d\xi^2} = \frac{d^2h}{d\xi^2}e^{\frac{-\xi^2}{2}} + \xi^2 u - 2\xi\frac{dh}{d\xi}e^{\frac{-\xi^2}{2}} - h(v)e^{\frac{-\xi^2}{2}} \tag{1.66}$$

$$\frac{d^2u}{d\xi^2} = [\frac{d^2h}{d\xi^2} + \xi^2 u - 2\xi\frac{dh}{d\xi} - h(v)]e^{\frac{-\xi^2}{2}} \tag{1.67}$$

Substituting Schrödinger equation for SHO :

$$(\xi^2 - \epsilon)h(\xi) = \frac{d^2h}{d\xi^2} + \xi^2 u - 2\xi\frac{dh}{d\xi} - h(v) \tag{1.68}$$

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\epsilon - 1)h = 0 \tag{1.69}$$

This form of Schrödinger equation is similar to the differential equation

$$\frac{d^2H_n}{d\xi^2} - 2\xi\frac{dH_n}{d\xi} + 2nH_n = 0 \tag{1.70}$$

Where H is known to be Hermite polynomials if n is an integer and $\epsilon - 1 = 2n$ is also integer.

Assume

$$h(\xi) = \xi^s \sum a_j \xi^j$$

We want find the second derivative of $h(\xi)$

The second derivative of the term $\frac{d^2H}{d\xi^2}$ is $(j+s)(j+s-1)a_j\xi^{j+s-2}$

The second derivative of the term $-2\xi\frac{dh}{d\xi}$ is $-2(j+s)a_j\xi^{j+s}$

The second derivative of the term $(\epsilon-1)h$ is $(\epsilon-1)a_j\xi^j$

substitute terms with ξ_j in equation 1.66, we have

$$\sum_{k=j}^{\infty}[(j+s)(j+s-1)a_j\xi^{j+s-2} - 2(j+s) + (\epsilon-1)a_j\xi^{j+s}] = 0 \tag{1.71}$$

Since the above is valid for all ξ, coefficients of each power of ξ can be equated to zero (uniqueness of power series expansions). Thus for $j = 0$and $j = 1$ we get two indicial equations,

$s(s-1)a_0 = 0$ if $a_0 \neq 0$ then $s = 0$ or $s = 1$

$s(s+1)a_0 = 0$ if $s = -1$ is not an acceptable condition since it introduces new singularity at $\xi = 0$

In general, for ξ^{j+s} ,

$$h(\xi) = \sum_{k=j}^{\infty} a_k \xi^{k+s}$$

$$(j+s+2)(j+s+1)a_j + 2 = (2j+2s+1-\epsilon a_j)$$

$$a_j + 2 = \frac{(2j+2s+1-\epsilon a_j)a_j}{(j+s+2)(j+s+1)}, j = 1, 2, 3, ...$$

There are two condition for solution $h(\xi) : (a_0, a_1)$, as $j \to \infty$,

$$\frac{a_{j+2}}{a_j} \cong \frac{2j}{j^2} = \frac{2}{j}$$

From Taylor series

$$e^{\xi^2} = \sum_{n=0}^{\infty} \frac{1}{n!} \xi^j, j = 0, 2, 4, ...$$

$$\text{let } c_j = \frac{1}{\frac{j}{2}!}$$

$$\frac{c_{j+2}}{c_j} = \frac{\frac{j}{2}!}{\frac{j+2}{2}|} = \frac{1}{\frac{j+2}{2}} = \frac{2}{2+j} \approx \frac{2}{j}$$

Hence asymptotically, $h(\xi)$ is behaving like e^{ξ^2} and, in turn $u(\xi)$ goes like $e^{\frac{\xi^2}{2}}$ something that we do not want as solution. Our requirement of normalizable solution can be met if the series is made to terminate, we choose $a_1 = 0$ then we have

$$a_3 = a_5 = a_7 = ... = 0$$

$$\exists j \ s.t. \ 2j + 1 = \epsilon \ , j = 0, 1, 2, \ldots$$

call $j = n$, where n is any integer , if we want take the odd numbers

$$\epsilon = 2n + 1 = \frac{2Em}{\hbar^2\alpha^2(n+\frac{1}{2})}, n = 1, 2, 3, ...$$

the energy eigenvalues of SHO are quantized and for $n = 0$ we have $E_0 = \hbar\omega^2$, as zero-point energy. The wave functions are :

$$u(\xi) = h(\xi)e^{\frac{\xi^2}{2}} = e^{\xi^2}\sum_{k=j}^{\infty} a_k\xi^k, \text{with}\frac{a_{j+2}}{a_j} = \frac{(2j + 2s - 2n)}{(j + 2)(j + 1)} \tag{1.72}$$

For the two solutions of the indicial equation , the wave functions are:

$$s = 0\ , u(\xi)_{even} = (a_0 + a_2\xi^2 + a_4\xi^4 + ... + a_n\xi^n)e^{-}\frac{\xi^2}{2}, n = 0, 2, 4, ... \tag{1.73}$$

$$s = 1\ , u(\xi)_{odd} = (a_0\xi + a_2\xi^3 + a_4\xi^5 + ... + a_n - 1\xi^{n-1})e^{-}\frac{\xi^2}{2}, n = 1, 3, 5, ... \tag{1.74}$$

The coefficients $a_0, a_2, a_4, ...$ in (1.73) are very different from those $a_0, a_2, a_4, ...$ in (1.74).

1.6 Potential

potential energy is the energy held by an object because of its position relative to other objects, stresses within itself, its electric charge, or other factors. There are different forms of potential energy : chemical potential energy : the energy which is stored in the bonds between the atoms , nuclear potential energy : is another stored form of potential energy in the nucleus, gravitational potential energy, elastic potential energy . Double well potential is one of a number of quartic potentials which contain two holes , the potential have two minima points . we can use Double-well potential as a model to explore various physical phenomena .

Exact solution for Schrödinger equation with double well potential cannot be easily find when using some potentials , so we have been using a developed technique to find the numerical solution like The finite element method (FEM). In this thesis, we solve the time independent schrödinger equation with double well potential to describe the behaviour the potential of nuclear attraction generated by two separate nuclei is given as :

$$\Psi = -e^{(-100((x-\frac{1}{4})^2+(y-\frac{1}{4})^2)-3)} - e^{(-100((x-\frac{3}{4})^2+(y-\frac{3}{4})^2)-3)}$$

We use the potential of the paper [1]. We use the double well potential for approximation the

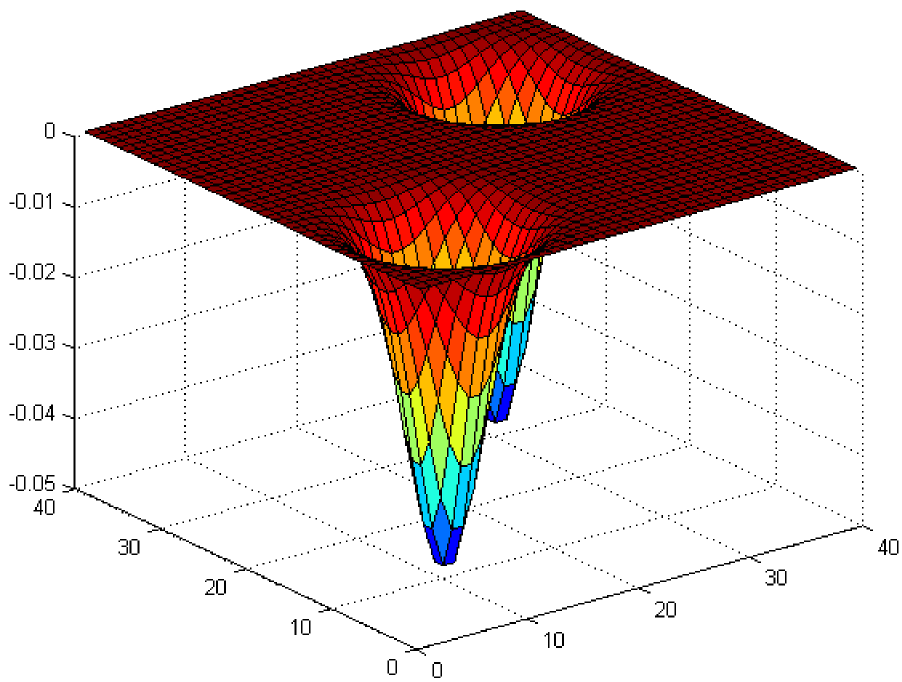

Fig. 1.1: the potential of nuclear attraction generated by two separate nuclei

partial differential equation which can not be solved analytically.

Chapter Two

Finite element method

In the FEM , the structural system is modeled by a set of appropriate finite elements interconnected at discrete points called nodes [4].
A node is a coordinate location in space where the degrees of freedom (DOFs) are defined. The DOFs for this point represent the possible movement of this point due to building the structure. Each linear triangular element has six degrees of freedom where the point has two degrees of freedom, the translation along X and Y axis. The basic building block of finite element analysis. There are several basic types of elements, including triangles and rectangles. Using the finite element approximation is feasible way in 2D to solve complex geometric domain. The main idea is, as in one-dimensional we divide the domain into cells and use polynomials for approximating a function over a cell.

2.1 Basis function

a basis function is a component of a specific basis for a function space. Each function in the function space can be represented as a linear combination of basis functions, there are many types of basis function some of this triangular elements, rectangular elements and basis spline. There are popular shapes of basis function Linear element, quadratic and cubic [2].

For an element with n nodes, $(n-1)$ order polynomial, the interpolation function is

$$N_k^e = \Pi_{i=1}^n \frac{x - x_i}{x_k - x_i}, K \mp i \tag{2.1}$$

we present linear element in one dimensional with i, j end nodes by

$$T(x) = \alpha_1 + \alpha_2 x \tag{2.2}$$

Where α_1 and α_2 are constants, we need two nodes to determine α_1 and α_2:

$$T_i = \alpha_1 + \alpha_2 x_i \tag{2.3}$$

$$T_j = \alpha_1 + \alpha_2 x_j \tag{2.4}$$

From the above equations, we obtain the following values

$$\alpha_1 = \frac{T_i x_j - T_j x_i}{x_j - x_i} \tag{2.5}$$

$$\alpha_2 = \frac{T_j - T_i}{x_j - x_i} \tag{2.6}$$

Substitute the values of α_1 and α_2 in equation 2.2

$$T = T_j[\frac{x - x_i}{x_j - x_i}] + T_i[\frac{x - x_j}{x_j - x_i}] \tag{2.7}$$

Then, we have:

$$T = T_j N_j + T_i N_i \tag{2.8}$$

where N_i and N_j are called Shape functions or Interpolation functions or Basis functions.

$$N_j = \frac{x - x_i}{x_j - x_i} \tag{2.9}$$

$$N_i = \frac{x_j - x}{x_j - x_i} \tag{2.10}$$

Two-dimensional linear triangular elements

A linear triangular element is a two-dimensional finite element that has three sides and three nodes have coordinates $(x_1\ \ y_1),\ (x_2\ \ y_2),\ (x_3\ \ y_3)$, each linear triangular element has six degrees of freedom where each node contributes two degrees of freedom. The two-dimensional linear triangular element, is represented by

$$T(x, y) = \alpha_1 + \alpha_2 x + \alpha_3 y \tag{2.11}$$

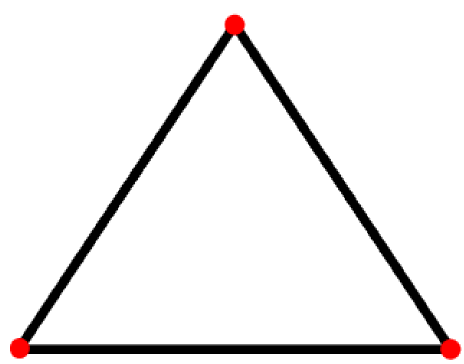

Fig. 2.1: A linear triangular element with three nodes

where the polynomials is linear in x and y contains three coefficients. We want to compute the displacement of the nodes at the triangle. We employ shape functions to insinuate the nodal displacements to calculate the displacements of arbitrary points within the triangles, we begin by moving only one point on the triangle and keep the other two fixed. The nodal displacements are

$$T_i = \alpha_1 + \alpha_2 x_i + \alpha_3 y_i$$

$$T_j = \alpha_1 + \alpha_2 x_j + \alpha_3 y_j$$

$$T_k = \alpha_1 + \alpha_2 x_k + \alpha_3 y_k \tag{2.12}$$

we can represented the above equations in the following matrix form

$$\begin{pmatrix} T_i \\ T_j \\ T_k \end{pmatrix} = \begin{bmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix}$$

Now solving for $\alpha_1,\ \alpha_2$ andα_3, we have

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{bmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{bmatrix}^{-1} \begin{bmatrix} T_i \\ T_j \\ T_k \end{bmatrix}$$

where

$$\begin{bmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{bmatrix}^{-1} = \frac{1}{2A} \begin{bmatrix} C_i & X_i & Y_i \\ C_j & X_j & Y_j \\ C_k & X_k & Y_k \end{bmatrix}^{T}$$

The area of a triangle is

$$A = \tfrac{1}{2} \times base \times height$$

$$2A = \det \begin{bmatrix} 1 & x_i & y_i \\ 1 & x_j & y_j \\ 1 & x_k & y_k \end{bmatrix} = (x_i\, y_j - x_j\, y_i) + (x_k\, y_i - x_i\, y_k) + (x_j\, y_k - x_k\, y_j)$$

Which results in the following:

$$\alpha_1 = \frac{1}{2A}[(x_j\, y_k - x_k\, y_j)T_i + (x_k\, y_i - x_i\, y_k)T_j + (x_i\, y_j - x_j\, y_i)T_k] \tag{2.13}$$

$$\alpha_2 = \frac{1}{2A}[(y_j - y_k)T_i + (y_k - y_i)T_j + (y_i - y_j)T_k] \tag{2.14}$$

$$\alpha_3 = \frac{1}{2A}[(x_k - x_j)T_i + (x_i - x_k)T_j + (x_j - x_i)T_k] \tag{2.15}$$

Substituting the values of $\alpha_1,\ \alpha_2$ and α_3 into equation 2.11 and collating the nodal displacements we get

$$T = N_i T_i + N_j T_j + N_k T_k = \begin{bmatrix} N_i & N_j & N_k \end{bmatrix} \begin{bmatrix} T_i \\ T_j \\ T_k \end{bmatrix} \tag{2.16}$$

Where

$$N_i = \tfrac{1}{2A}(a_i + b_i x + c_i y)$$
$$N_j = \tfrac{1}{2A}(a_j + b_j x + c_j y)$$
$$N_k = \tfrac{1}{2A}(a_k + b_k x + c_k y)$$

and

$$a_i = x_j\, y_k - x_k\, y_j;\ b_i = y_j - y_k;\ c_i = x_k - x_j$$

$$a_j = x_k\, y_i - x_i\, y_k;\ b_j = y_k - y_i;\ c_j = x_i - x_k$$

$$a_k = x_i\, y_j - x_j\, y_i;\ b_k = y_i - y_j;\ c_k = x_j - x_i$$

If we evaluate N_i at node i, where the coordinates are (x_i, y_i), then we obtain

$$(N_i)_i = (x_j\, y_k - x_k\, y_j) + (y_j - y_k)x_i + (x_k - x_j)y_i = \frac{2A}{2A} = 1 \qquad (2.17)$$

In the same way we can proof that $(N_j)_i = (N_k)_i = 0$. Thus, the shape functions have a value of unity at the designated vertex and zero at all other vertices. It is possible to show that

$$N_i + N_j + N_k = 1 \qquad (2.18)$$

Everywhere in the element, including the boundaries.

Two-dimensional rectangular elements

rectangular element is a type of element used in FEM which is used to approximate in a 2D domain the exact solution of Schrödinger equation. The rectangular element has four nodes and the nodes have coordinates (x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4) in each corner. The general approximation over a rectangular element is

$$T = \alpha_1 + \alpha_2\, x + \alpha_3\, y + \alpha_4\, x\, y \qquad (2.19)$$

Fig. 2.2: A simple rectangular element with four nodes

On substituting the displacements of the nodes $T_1,\ T_2,\ T_3\ and\ T_4$ into equation 2.21, we obtain the values of $\alpha_1,\ \alpha_2,\ \alpha_3\ and\ \alpha_4$. Substituting these relationships into equation 2.21 and collating the coefficients of $T_1, T_2, ..., T_4$, we get

$$T = N_1T_1 + N_2T_2 + N_3T_3 + N_4T_4 \tag{2.20}$$

where for a rectangular element, the shape functions

$$N_1 = \tfrac{1}{4ab}\,(b-x)(a-y)$$
$$N_2 = \tfrac{1}{4ab}\,(b+x)(a-y)$$
$$N_3 = \tfrac{1}{4ab}\,(b+x)(a+y)$$
$$N_4 = \tfrac{1}{4ab}\,(b-x)(a+y)$$

The shape functions can also be obtained using Lagrange interpolation functions.

Definition 2.1.1 *An operator T is amapping(function)*

$T\ :\ X \to Y$

where $x,\ y$ metric spaces or normed spaces .

Definition 2.1.2 *Let X be a vector space over the complex numbers C. An inner product on X is a mapping $(.,.)_x\ :\ X \times\ X \to\ C$ such that :*

- $(x,x)_x \geq 0$, $(x,x)_x = 0$ *iff* $x = 0$

- $\overline{(x,y)_x} = (y,x)_x$ *for all*$x, y \in X$

- *for all* $x,\ y,\ z\ \in\ X$*and* $\alpha\ ,\beta\ \in\ C$ *we have that*

  $(\alpha x + \beta y, z)_x = \alpha(x,z)_x + \beta(y,z)_x$ *for simplicity we write the inner product as* $(.,\ .)$ *. the inner product induces a norm on* X *:* $||x||_x = \sqrt{(x,x)_x} for\ all\ x \in X$

Definition 2.1.3 *A complete inner product space X is called a Hilbert space.*

Linear operator : Let X and Y be normed spaces. An operator $T : X \to Y$ is said to be linear if

$$T(\alpha x_1 + \beta x_2) = \alpha T x_1 + \beta T x_2$$

for all $\alpha \, , \beta \, \in \, C$ and $x_1, x_2 \, \in X$

Notation

$N_o = N \cup 0$

For an open set $\Omega \subseteq Rm$,

$C(\Omega)$: space of all continuous real valued functions on Ω.

$C_0(\Omega)$: set of all functions in $C(\Omega)$ with compact support.

$C^k(\Omega)$: the set of k times continuously differentiable functions on Ω.

$C_0^k(\Omega)$: the set of k times continuously differentiable functions with compact support in Ω.

$c_0^\infty(\Omega)$: the set of smooth function, i.e., infinite times continuously differentiable functions with compact support in Ω.

$L^p(\Omega)$: the set of functions s.t. $\int |\emptyset|^p dx < \infty$, where $|\emptyset|^p$ is integrable when $p = 2$ we have $L^2(\Omega)$ equipped inner product then

$$(u, v)_{L^2} = uvdx \tag{2.21}$$

We use $||.||$ instead of $||.||_{L^2}$

Definition 2.1.4 ***The Sobolev spaces***

The variational theory and convergence analysis of finite element methods relies on the notions of Sobolev spaces.[5] The Sobolev spaces are defined as $W^{s,p}(\Omega) = f \in L^p(\Omega)$ for all $|\alpha| \leq s, \; 1 \leq p < \infty$ where s is anonnegative integer and $|\alpha| = \sum_{i=1}^n \alpha_i, \; i = 1, \; 2, \; 3, \; ... \; n$ with non-negative integer components α_i $W_0^{s,p}(\Omega)$: the closure of $C_0^\infty(\Omega)$ in the $W^{s,p}(\Omega)$

norm. when $p = 2$ *we have* $W^{s,2}(\Omega)$ *we denote by* $H^s(\Omega)$ *and* $H_0^s(\Omega) = W_0^{s,p}(\Omega)$ *we use* $||\,.\,||_{H^s}$ *instead of* $||\,.\,||_{W^{s,2}(\Omega)}$.

2.2 Finite Element Method construction

The time-independent Schrödinger equation with a potential Ψ of the form:

$$Hu := -\Delta u + \Psi u = Eu,\ \text{in}\Omega \tag{2.22}$$

$$u = 0,\ \text{on}\ \partial\,\Omega$$

where $\Omega \in \mathbb{R}^{\partial}$ is abounded domain $\partial\Omega$, the weak form of the eigenvalue problem of Schrödinger equation is :

$$a(u, v) = \lambda(u, v)\ \text{for all}\ v \in V \tag{2.23}$$

Where $V := u : u \in H_0^1(\Omega)\ ,\ u|_{\partial\Omega} = 0$ and $H_0^1 \subseteq H^1$ the space of all functions that vanishes on $\partial\Omega$ in the Sobolev space. Let $\{\varphi 1,\ \varphi 2, ...,\ \varphi N\ \}$ be the basis functions of the linear Lagrange element space V_h and

$$u_h = \textstyle\sum_{i=1}^{N} u_i \varphi_i$$

where $u_i \in \mathbb{R}$ are the unknown coefficients . The discretized form of the finite eigenvalue problem is obtained as follows: to find a finite eigenvalue problem $\lambda \in \mathbb{R}$ and $u_h \in V_h$ for all $v_h \in V_h, V_h \subseteq V$

$$a(u_h, v_h) = \lambda_h(u_h, v_h) \tag{2.24}$$

Substituting u_h in equation 2.24 and choosing $v_h = \varphi_j$ we have:

$$a(\sum_{i=1}^{N} u_i\varphi_i, \varphi_j) = \lambda_h(\sum_{i=1}^{N} u_i\varphi_i, \varphi_j),\ j = 1, ..., N$$

We want to use the definition of $a(.\ ,\ .)$ where $u,\ v \in V_h$

$$a(u, v) := (\nabla u, \nabla v)$$

$$\sum_{i=1}^{N} (\nabla\varphi_i, \nabla\varphi_j)u_i = \lambda_h \sum_{i=1}^{N} (\varphi_i, \varphi_j)\, u_i,\ J = 1, ..., N \tag{2.25}$$

The matrix form of the above linear system is given by

$$Au = \lambda_h Mu$$

Where A and M are the N $\times$ N stiffness matrix and mass matrix given by

$$A_{i,j} = \big(\nabla\varphi_i, \nabla\varphi_j\big)$$
$$M_{i,j} = (\varphi_i, \varphi_j)$$

Where A and M are the N $\times$ N stiffness matrix and mass matrix. Now, we want to compute the local stiffness where is relates the traction components at the inner and outer surface of agiven element to the corresponding displacements and also we want to compute the mass matrix which is a symmetric matrix expresses the multiplication for the quadrature points of the triangular elements, and we want distribute the local stiffness matrix and mass matrix to the global stiffness and mass matrices.

Let K be a triangle of the mesh whose vertices are I, J, Lin "p", which are the global indices. In other words, the global basis functions $\varphi_I, \varphi_J, \varphi_L$ have K as part of their support. Locally, we give indices $1, 2, 3$ to these vertices such that we have the so-called local-to-global mapping $1 \leftrightarrow I, 2 \leftrightarrow J, 3 \leftrightarrow L$ the restriction of the basis function $\varphi_I, \varphi_J, \varphi_L$ on K by $\varphi_1, \varphi_2, \varphi_3$. Now , the local stiffness matrix is given by

$$A_{local} = \begin{pmatrix} (\nabla\varphi_1\nabla\varphi_1)_K & (\nabla\varphi_2,\nabla\varphi_1)_K & (\nabla\varphi_3,\nabla\varphi_1)_K \\ (\nabla\varphi_1,\nabla\varphi_2)_K & (\nabla\varphi_2,\nabla\varphi_2)_K & (\nabla\varphi_3,\nabla\varphi_2)_K \\ (\nabla\varphi_1,\nabla\varphi_3)_K & (\nabla\varphi_2,\nabla\varphi_3)_K & \nabla\varphi_3,\nabla\varphi_3)_K \end{pmatrix}$$

Let the coordinates of the vertices of K be given by $x1,\ y1,\ x2,\ y2,\ x3,\ y3$ Recall that the vertices of k are $(0,\ 0), (1,\ 0), (0,\ 1)$. The linear basis functions on $\hat{K}$ are simply

$$\hat{\varphi}_1\ =\ 1 - x - y, \hat{\varphi}_2 = x, \hat{\varphi}_3 = y$$

Their gradients are given by

$$\nabla\hat{\varphi}_1 = \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \nabla\hat{\varphi}_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \nabla\hat{\varphi}_3 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

the local stiffness matrix and mass matrix for k are

$$\frac{1}{2}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \frac{1}{2}\begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{pmatrix}$$

Here $\frac{1}{2}$ is the area of the reference triangle k . The affine mapping from $\hat{k}$ to k is defined as $F : k \rightarrow K$such that $Fx := B\hat{x} + b$, where

$$B = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{pmatrix} \text{ and } b = \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}$$

If $\hat{p}$ is a scalar function, we obtain a function p on k by $F\hat{x} := Bx+b$, In particular, the basis functions $\hat{\varphi}_1$, $\hat{\varphi}_2$, $\hat{\varphi}_3$are transformed to $\varphi_1, \varphi_2, \varphi_3$ The gradient transforms as $(\nabla p)oF = (B^{-1})^T \nabla \hat{p}$ where ∇ is with respect to x. Quadratures of triangle is

$$\int f(x)dx \approx \frac{1}{2} \sum_{i=1}^{q} w_i f(x_i) \tag{2.26}$$

where $w_i's$ are weight and $x_i's$ are quadrature points for the refences triangle $\hat{k}$

let $\hat{K} = 1 : \int f(x)dx \approx |K| f(a^{123})$ where a^{123} abarycenter point

l et $\hat{K} = 2 : \int f(x)dx \approx \sum_{1\leq i<j\leq 3} f(a^{ij}) \frac{|K|}{3}$

For local stiffness matrix, the values of the gradients of the basis functions at a_{12}, a_{23}, a_{31} can be obtained from the corresponding values for the reference triangle k , we have that

$$(\nabla\varphi_1, \nabla\varphi_2) = \int \nabla\varphi_1.\nabla\varphi_2 dx \tag{2.27}$$

$$(\nabla\varphi_1, \nabla\varphi_2) = \sum_{1\leq i<j\leq 3} \nabla\varphi_1(a^{ij}).\nabla\varphi_2(a^{ij}) \frac{|K|}{3} \tag{2.28}$$

$$(\nabla\varphi_1, \nabla\varphi_2) = \sum_{1\leq i<j\leq 3} [B^{-T}\nabla\varphi_1(a^{ij})].[B^{-T}\nabla\varphi_2(a^{ij})] \frac{|K|}{3} \tag{2.29}$$

$$(\nabla\varphi_1, \nabla\varphi_2) = |K| [B^{-T} \begin{pmatrix} -1 \\ \\ -1 \end{pmatrix}][B^{-T} \begin{pmatrix} 1 \\ \\ 0 \end{pmatrix}] \tag{2.30}$$

We want find the quadrature points in the triangle K which have vertices (0,0) in point 1 (1,0) in point 2 (0,1)in point 3

$a^{12} = ((\frac{1}{2}), 0), a^{13} = (0, \frac{1}{2}), a^{23} = (\frac{1}{2}, \frac{1}{2})$

the basis function on the quadrature points are

$\hat{\varphi}_1(a^{12}) = 1 - x - y = 1 - \frac{1}{2} - 0 = \frac{1}{2}$

$\hat{\varphi}_1(a^{13}) = 1 - x - y = 1 - 0 - \frac{1}{2} = \frac{1}{2}$

$\hat{\varphi}_1(a^{23}) = 1 - x - y = 1 - \frac{1}{2} - \frac{1}{2} = 0$

$\hat{\varphi}_2(a^{12}) = x = \frac{1}{2}$

$\hat{\varphi}_2(a^{13}) = x = 0$

$\hat{\varphi}_2(a^{23}) = x = \frac{1}{2}$

The mass matrix

$$(\varphi_1, \varphi_2) = \frac{|K|}{3} \sum_{1 \leq i < j \leq 3} \hat{\varphi}_1(a^{ij}).\hat{\varphi}_2(a^{ij}) \tag{2.31}$$

$$(\varphi_1, \varphi_2) = \tfrac{|K|}{3}[\hat{\varphi}_1(a^{12}).\hat{\varphi}_2(a^{12}) + \hat{\varphi}_1(a^{13}).\hat{\varphi}_2(a^{13}) + \hat{\varphi}_1(a^{23}).\hat{\varphi}_2(a^{23})]$$

$$(\varphi_1, \varphi_2) = \frac{|K|}{3}[\frac{1}{2}.\frac{1}{2} + 0.\frac{1}{2} + \frac{1}{2}.0] = \frac{|K|}{12} \tag{2.32}$$

Chapter Three

Numerical Implementation

we use Matlab program to solve the time-independent Schrödinger equation with double-well potential Ψ and find the eigenvalues and the eigenfunctions and compute the error results of eigenvalue. we choose 3 different domain in 2D to examine the behaviour of such equations when solved on domains with different geometrical shape

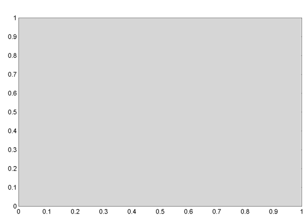

Fig. 3.1: Square domain in example 4.0.1

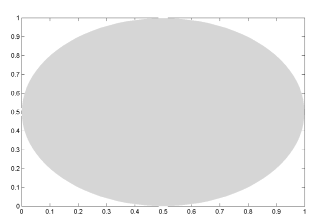

Fig. 3.2: Circle domain in example 4.0.2

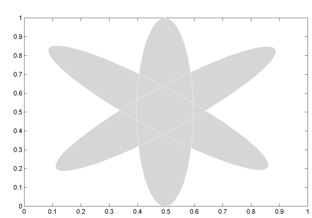

Fig. 3.3: Star domain in example 4.0.3

We solve the time-independent Schrödinger equation on different levels of refinement by using FEM. **Examples**

Example 3.0.1 *we consider the Schrödinger equation(3.1) on the square domain* $\Omega \subseteq [0,1]^2$ *and the potential* $\Psi = -e^{(-100((x-\frac{1}{4})^2+(y-\frac{1}{4})^2)-3)} - e^{(-100((x-\frac{3}{4})^2+(y-\frac{3}{4})^2)-3)}$

to solve this example we use the Matlab program by using the code pdetool to apply the Finite Element Method, we repeat the iteration five times. As a result of that we obtain five different degrees of freedom and we compute the relative error of the eigenvalues. at the end of solving the Schrödinger equation by Finite Element Method we obtain the eigenfunctions as shown in the figures.

Tab. 3.1: Relative error and the first eigenvalue for Schrödinger eigenvalue problem in Example 4.0.1 using FEM

	d.f	Elements	eigenvalue	relative error
1	184	326	20.061251	-
2	693	1304	19.915973	0.00729454694
3	2689	5216	19.879115	0.00185410668
4	10593	20864	19.869843	0.000466636802
5	42049	83456		0.000116974847

In the first iteration of the first eigenvalue, we have 184 degree of freedom and the eigenvalue is 20.061251 when we did the mesh again we have 693 and the relative error is 0.00729454694 when we repeat the mesh for the third time we have 2689 degree of freedom and the relative error is 0.00185410668 as shown in the table. we notice that When we refinement the mesh the degrees of freedom are increased and the relative error is decreased. As a result for that , we conclude that the eigenvalue 19.869843 is the best than other values.
the next of two examples, we use the same procedures that we used in this example.

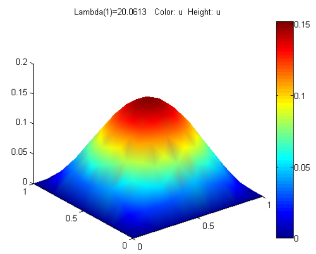

Fig. 3.4: Eigenfunction with d.f 184and $\lambda1=20.061251$

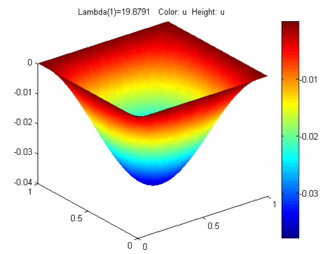

Fig. 3.5: Eigenfunction with DOF 2689 and $\lambda1=19.879115$

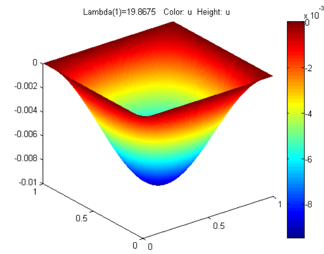

Fig. 3.6: Eigenfunction with DOF 42049 and $\lambda1=19.867519$

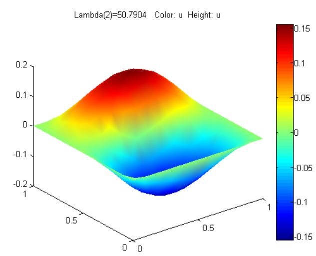

Fig. 3.7: Eigenfunction with DOF 184 and $\lambda2=50.790380$

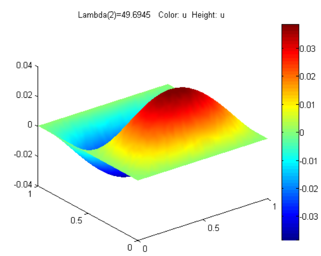

Fig. 3.8: Eigenfunction with DOF 2689 and $\lambda2=49.694529$

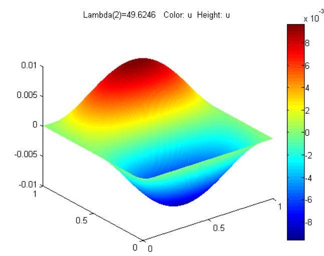

Fig. 3.9: Eigenfunction with DOF 42049 and $\lambda2=49.624628$

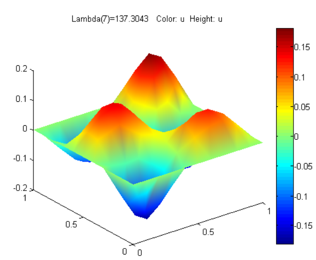

Fig. 3.10: Eigenfunction with DOF 184 and $\lambda3=137.304254$

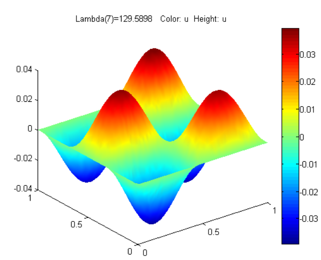

Fig. 3.11: Eigenfunction with DOF 2689 and $\lambda3=129.589770$

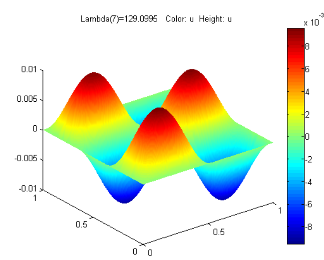

Fig. 3.12: Eigenfunction with DOF 42049 and $\lambda3=129.099510$

Fig. 3.13: Corresponding eigenfunction for anumber of eigenvalues in Example 4.0.1

when the degrees of freedom is increased the accurate of eigenfunctions is increased as shown in figure 3.13.

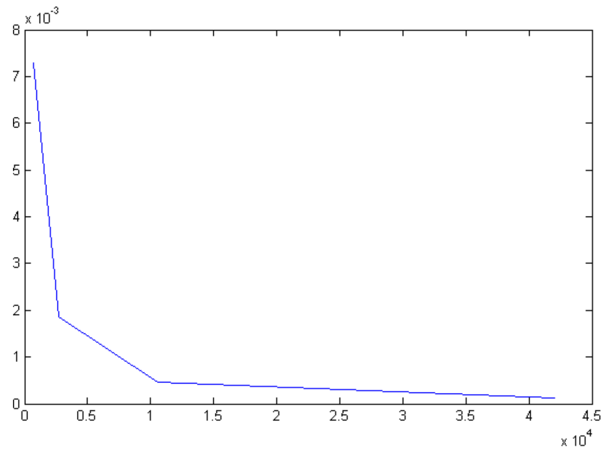

Fig. 3.14: Degrees of Freedom and relative error of the first eigenvalue on example 4.0.1

Example 3.0.2 *In this example, we consider the Schrödinger equation(3.1) on the circle domain $\Omega \subseteq [0,1]^2$ and the potential* $\Psi = -e^{(-100((x-\frac{1}{4})^2+(y-\frac{1}{4})^2)-3)} - e^{(-100((x-\frac{3}{4})^2+(y-\frac{3}{4})^2)-3)}$

Tab. 3.2: Relative error and the first eigenvalue for Schrödinger eigenvalue problem in Example 4.0.2 using FEM

	d.f	Elements	eigenvalue	relative error
1	153	272	23.449111	-
2	577	1088	23.239150	0.00903479688
3	2241	4352	23.186075	0.00228908946
4	8833	17408	23.172739	0.000575503828
5	45073	69632	23.169399	0.00014415566

In the first iteration of the first eigenvalue on the circle domain, we have 153 degree of freedom and the eigenvalue is 23.449111 when we did the mesh again we have 577 and the relative error is 0.00903479688 when we repeat the mesh for the fifth time we have 45073 degree of freedom and the relative error is 0.00014415566 ,sothe eigenvalue 23.169399 is the best value than other values because it has the biggest degree of freedom value and the lowest error value .

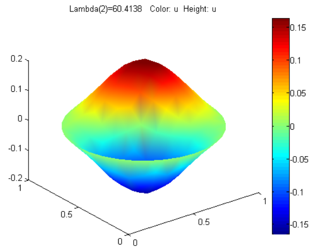

Fig. 3.15: Eigenfunction with DOF 272 and λ1 =23.449111

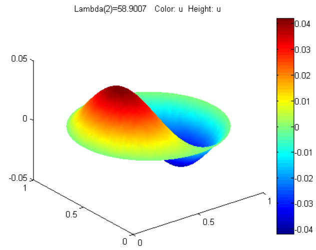

Fig. 3.16: Eigenfunction with DOF 4352 and λ1=23.186075

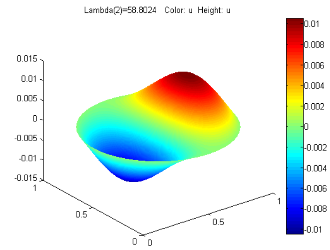

Fig. 3.17: Eigenfunction with DOF 69632 and λ1=23.169399

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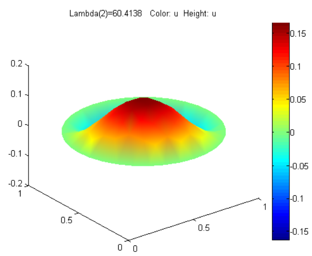

Fig. 3.18: Eigenfunction with DOF 272 and λ2=60.413758

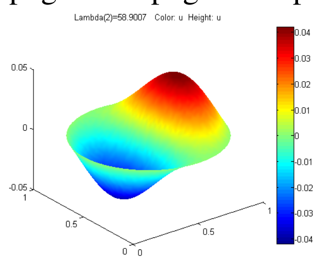

Fig. 3.19: Eigenfunction with DOF 4352 and λ2=58.900651

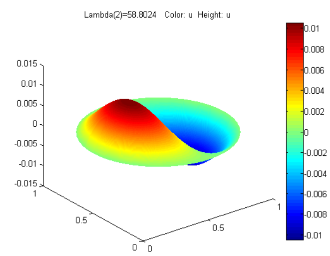

Fig. 3.20: Eigenfunction with DOF 69632 and λ2=58.802428

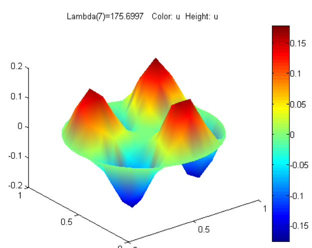

Fig. 3.21: Eigenfunction with DOF 272 and λ3=175.699651

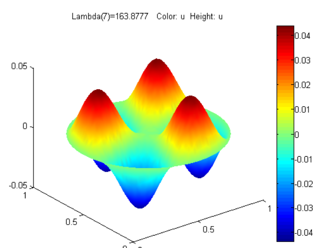

Fig. 3.22: Eigenfunction with DOF 4352 and λ3=163.877746

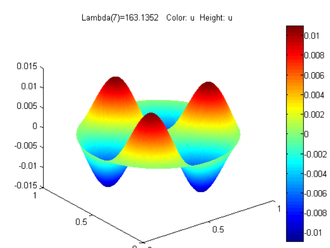

Fig. 3.23: Eigenfunction with DOF 69632 and λ3=163.135213

Fig. 3.24: Corresponding eigenfunction for a number of eigenvalues in Example 4.0.2

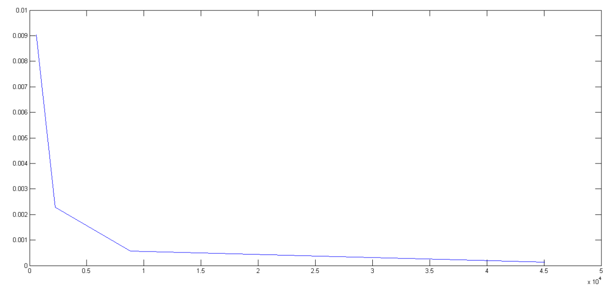

Fig. 3.25: Degrees of Freedom and relative error of the first eigenvalue on example 4.0.1

Example 3.0.3 *In this example, we consider the schrodinger equation(3.1) on the circle domain* $\Omega \subseteq [0,1]^2$ *and the potential* $\Psi = -e^{(-100((x-\frac{1}{4})^2+(y-\frac{1}{4})^2)-3)} - e^{(-100((x-\frac{3}{4})^2+(y-\frac{3}{4})^2)-3)}$

Tab. 3.3: Relative error and the first eigenvalue for Schrödinger eigenvalue problem in Example 4.0.2 using FEM

	DOF	Elements	E_1	relative error
1	183	299	118.256173	-
2	664	1196	111.865048	0.0571324566
3	2523	4748	109.620591	0.0204747756
4	9829	19146	108.790140	0.00763351348
5	38793	76544	108.468500	0.00296528485

The eigenvalue of the fifth-iteration of the refinement mesh is the best.

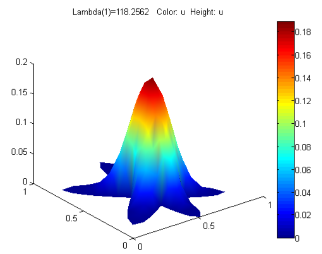

Fig. 3.26: Eigenfunction with DOF 183and λ1=118.256173

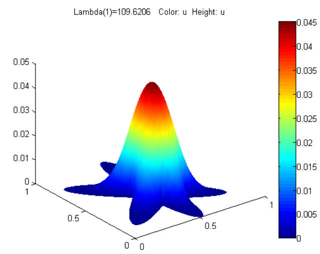

Fig. 3.27: Eigenfunction with DOF 2523 and λ1=109.620591

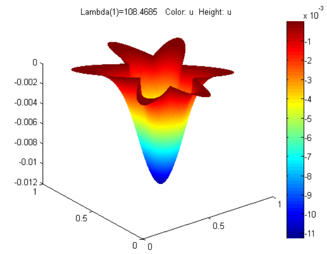

Fig. 3.28: Eigenfunction with DOF 38793 and λ1=108.468500

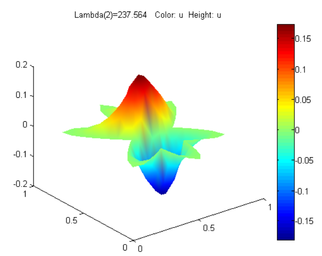

Fig. 3.29: Eigenfunction with DOF 183 and λ2=237.564034

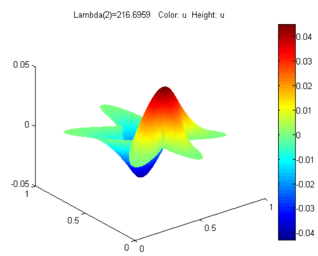

Fig. 3.30: Eigenfunction with DOF 2523 and λ2=216.695905

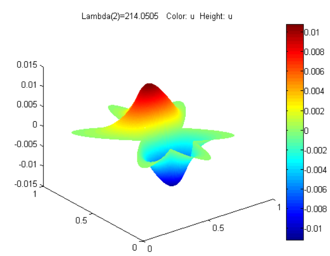

Fig. 3.31: Eigenfunction with DOF 38793 and λ2=214.050513

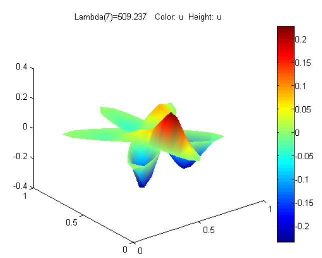

Fig. 3.32: Eigenfunction with DOF 183 and λ3=509.237011

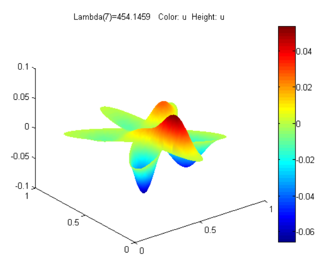

Fig. 3.33: Eigenfunction with DOF 2523 and λ3=454.145900

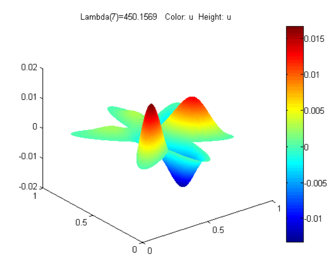

Fig. 3.34: Eigenfunction with DOF 38793 and λ3=450.156901

Fig. 3.35: Corresponding eigenfunction for anumber of eigenvalues in Example 4.0.3

The figures show the first ,third and the seventh eigenfunctions for corresponding eigenvalues for different level of mesh refinement which are the first ,third and fifth level of mesh in the fifth iteration the shapes of eigenfunction are smoothly than the first and third iteration.

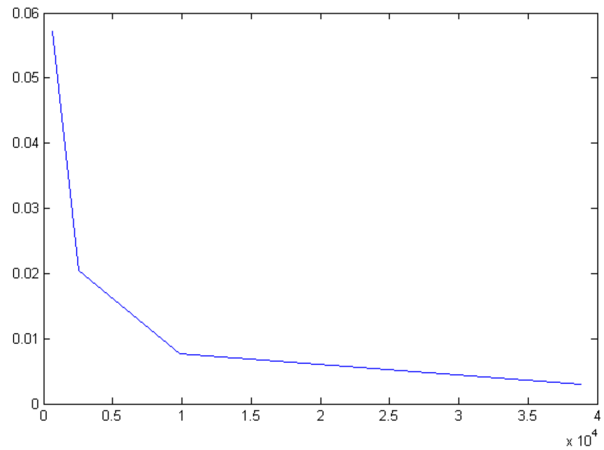

Fig. 3.36: Degrees of Freedom and relative error of the first eigenvalue on example 4.0.3

We notice that the relationships between Degrees of Freedom and relative error is negative. We illustrate the result by used PDE tool in Matlab program. FEM solved and approximation the time independent Schrödinger equation through discretization the domain into element and refinement the mesh to gave us the eigenvalues and eigenfunctions as shown in the above tables and figures.

Chapter Four

conclusion

In this thesis, we consider the finite element method to solve the Schrödinger equation with double-well potential to find the eigenvalues and corresponding eigenfunctions and we used the Matlab program to apply The Finite Element method on three forms of the domain and solve Schrödinger equation to gave us the eigenvalues and eigenfunctions. we compute the relative error between the eigenvalues and we conclude that the accurate increase when the refinement iteration or the Degree of Freedom is increase. In further studies we will expand our framework to solve Schrödinger equation in 3D and we will try to test higher order elements such as quadratic elements and compare the results with linear elements used in this thesis.

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الملخص

استخدام طريقة العناصر المحدودة لحل مشكلة القيمة الذاتية لمعادلة شرودنغر في بعدين

تعتبر طريقة العناصـــر المحدودة تقنية معروفة لحل المعادلات التفاضـــلية الجزئية عدديا. كما تم تطويره في الأصل لحل المشكلات التي تحدث في الهندسة والفيزياء الرياضية. علاوة على ذلك ، فهي طريقة رقمية لحل المشـــكلات المعقدة مثل التحليل الهيكلي ونقل الحرارة وتدفق الســـوائل والأنظمة المعقدة.

في طريقة العناصـر المحدودة، نقسـم المجال في اتجاه واحد إلى خلايا ونسـتخدم متعددات الحدود لتقريب دالة فوق خلية. بينما ، إذا كان المجال يحتوي على اتجاهين ، فإننا نقســـمه إلى نطاقات فرعية فواصل زمنية وتمييز نظام معين إلى أجزاء أصغر وأبسط تسمى العناصر وهذه متصلة بالعقد ونختار وظائف الأســاس لتوفير تقريب للحل غير المعروف داخل عنصــر. تؤدي صــياغة طريقة العناصــــر المحدودة لمشـــكلة القيمة الحدية أخيرا إلى نظام من المعادلات الجبرية. ثم يتم تجميع المعادلات البســيطة التي تشــكل هذه العناصــر المحدودة في نظام أكبر من المعادلات التي تشكل المشكلة بأكملها. ثم تقوم طريقة العناصر المحدودة بتقريب الحل عن طريق تقليل دالة الخطأ المرتبطة عبر حســاب التفاضــل والتكامل للاختلافات. تحتوي الدوال الأســاســية على ثلاثة أنواع مختلفــة من العنــاصــــر وهي الخطيــة والعنــاصــــر التربيعيــة والعنــاصــــر المكعبــة. في هذا العمل، نستخدم فقط العناصر الخطية لأنها أسرع من غيرها. نحن نطبق طريقة العناصر المحدودة ذات الإمكانات الجيدة المزدوجة باســـتخدام ثلاثة مجالات مختلفة. في نهاية الأطروحة ، نعطي أمثلة رقمية ذات مجالات مختلفة.