NUMERICAL SOLUTION OF SCHRODINGER'S EQUATION BY LOBATTO QUADRATURE METHOD OF SIXTH ORDER

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Numerical Solution Of Schrodinger's Equation By Lobatto Quadrature Method Of Sixth Order

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DECLARATION

I, the undersigned, declare that this project is my original work and the result of my own investigations, except as acknowledged, to the best of my knowledge and belief, has not been presented for award of a degree in University of Nairobi or any other University.

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Declaration by the Supervisor

This project report has been submitted for examination with my approval as the supervisor.

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Date: .....

STATEMENT

This dissertation has been submitted in partial fulfilment of requirements for a Master of Science degree at the University of Nairobi and is deposited in the University Library to be made available to borrowers under the rules and regulations of the Library.

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ABSTRACT

The one dimensional time independent Schrodinger's equation is a second order boundary value problem without the first order term explicitly. In this current study, the solution of the time independent Schrodinger's equation is obtained using the Wood's - Saxon Potential. The computation is done numerically by using a sixth order method based on Lobatto quadrature. This generates the different values of energies for the first six bound states after the same number of iterations as that of Numerov's method. The results obtained by Lobatto quadrature formula are compared against those for Numerov's method for the various values of the step lengths. This is done in terms of computation of the errors with respect to the analytical solutions. The magnitude of the errors for both methods indicates that Lobatto quadrature method yield values which have smaller errors than Numerov's method when compared with the exact solutions.

DEFINITION OF TERMS

i ***Forward difference***

It is a finite difference given by;

$$\Delta[f_k] = f_{k+1} - f_k$$

ii ***Backward difference***

It is given by;

$$\nabla[f_k] = f_k - f_{k-1}$$

iii ***Central difference operator***

It is a difference operator denoted by;

$$\delta[f_k] = f_{\left(k+\frac{1}{2}\right)} - f_{\left(k-\frac{1}{2}\right)}$$

iv ***Work function,*** $\mathbf{W_0}$

It is the minimum amount of energy that is needed to dislodge an electron from a certain metal surface.

v ***Threshold frequency,*** $\mathbf{f_0}$

The minimum frequency of a radiation that is needed to eject an electron from a certain metal surface.

vi ***Momentum ,*** **p**

It is the product of linear velocity and mass.

CHAPTER 1

INTRODUCTION

1.1 Background of Boundary Value Problems

1.1.1 Introduction

Numerical solution procedures occupy an extremely important part in many areas of sciences. These include engineering, astrophysics, laser physics, nuclear reaction, highly oscillatory motions in bodies, atomic and nuclear scattering problems, molecular-dynamics calculations for liquids and gases, stellar mechanics and pollution of the atmosphere. In most areas, where there is a quantitative component, there is always great interest in describing how systems evolve with time, that is, in describing the dynamics of a system. In the simplest one-dimensional case, the state of a system at any time, t, is denoted by a function which is generally written as $u = u(t)$. Considering u, a dependent variable, knowing it is important in order to know the state that the system is in, at any time, t. For example, $u(t)$, could be the population of an animal species in an ecosystem, the concentration of a chemical substance in the blood, the number of infected individuals in a flu epidemic, the current in an electrical circuit among others. The differential equation describes how a state changes. Many models are in form of dynamic equations that relate the state, $u(t)$, to its rates of change as expressed by its derivatives, $u'(t)$, $u''(t)$, ...and so on. Such equations are called differential equations and many laws of nature take the form of such.

Explicit solutions when known can be used as test cases for tracking the reliability and accuracy of a chosen numerical scheme. Thus the classification of equilibrium and their stability properties as well as first intervals and Lyapunov functions play an important role. This leads to the boundary value problem which is a field of differential equations.

A boundary value problem is a differential equation together with a set of additional constraints called the boundary conditions. A solution to a boundary value problem satisfies the boundary conditions.

The boundary value problem described in this case is a two-point boundary value problem. A two point boundary value problem of total order n on a finite interval $[a, b]$ may be written as an explicit first order system of ordinary differential equations with boundary values evaluated at two points as;

$$y''(x) = f[x, y(x)], x \in (a, b) \tag{1.1}$$

$$g(y(a), y(b)) = 0$$

Here $y, f, g \in \Re^n$ and the system is called explicit. The n boundary conditions defined by g must be independent that is they cannot be expressed in terms of each other. There are four types of boundary value problem depending on the boundary conditions set. These are;

i) Dirichlet boundary condition

Also known as the first-type, is a type of boundary condition named after Peter Gustar Lejeune Dirichlet. When imposed on an ordinary or partial differential equation, it specifies the values that a solution needs to take on along the boundary of the domain. Given an ordinary differential equation;

$$y'' + y = f(x, y)$$

the Dirichlet conditions on the interval [a,b] take the form:

$y(a) = \alpha$ and $y(b) = \beta$ where α and β are given numbers.

ii) Neumann boundary condition

Also known as the second boundary condition was was named after Calr Neumann. When imposed on an ordinary or partial differential

equation it specifies the values that the derivatives of a solution has taken on the boundary of the domain. For an ordinary differential equation for instance;

$$y'' + y = f(x, y)$$

,

The Neumann boundary conditions on the interval [a,b] take the form $y'(a) = \alpha$ and $y'(b) = \beta$ where α and β are given numbers.

iii) Robin boundary condition

Also known as the third type boundary condition is a boundary condition named after Victor Gustare Robin. When imposed on an ordinary or a partial differential equation, it is a specification of a linear combination of the values of a function and its derivative on the boundary of the domain. It is therefore a weighted combination of Dirichlet and Neumann boundary condition. Given that a and b are allowed to be functions, rather than constants in an example, $\Omega = [0, 1]$, the Robin boundary becomes the conditions:

$$ay(0) + by'(0) = f(0)$$

$$ay(1) + by'(1) = f(1)$$

for a given differential equation.

iv) Cauchy boundary condition

A Cauchy boundary condition named after Louis Cauchy specifies both the function value and the normal derivative on the boundary of the domain. They are common in second order ordinary differential equations; $y''(x) = f(x)$.

In order to ensure that a unique solution $y(x)$ exists, one specifies the value of the function y and the value of the derivative y' at a given point, say $x = a$. For instance $y(a) = \alpha$ and $y'(a) = \beta$ where a is a boundary value.

1.1.2 Phenomena giving rise to boundary value problems

In the current research, I consider the second order boundary value problem where the first order derivative does not appear explicitly. It occurs in a number of cases outlined below.

1 Newton's Mechanics

If the force F(x,t) acting on a particle is known, then one can write a second order differential equation to find $x(t)$. For instance; $F(x,t) = ma$ (Newton's Second law of motion).

$$F(x,t) = m\frac{d^2y(t)}{dx^2} \tag{1.2}$$

which is second law of Newtonian mechanics. This law relates the force, mass and acceleration of an object whose position is $x(t)$ at time, t. Force applied to an object is equal to its mass, m times its acceleration $\frac{d^2y}{dx^2}$.

A physical phenomenon involving this is when the trajectory of a vertically projected object is considered between the point of projection and landing. Hence, its height above the point of projection at any time is given by $x(t_0) = x(t_n) = 0$ where t_0 and t_n represents the time at point of projection and landing respectively.

2 Spring's and Hooke's law

For Hooke's law provided the force, y is not so large not to deform the spring then the restoring force $F_{spring} = -ky$ where $k > 0$ is a constant depending on the properties of the spring.

Combining Hooke's law and Newton's second law of motion implies

$m\frac{d^2y}{dx^2} = -ky$ for $m = 0$

$\frac{d^2y}{dx^2} = -\frac{ky}{m} \Rightarrow \frac{d^2y}{dx^2} = -\omega^2 y$

where $\omega^2 = \frac{k}{m}$

Let $u(x)$ denote the position of a string at x which is specified and

depends on $f(x)$. Considering balance of the force, we get a differential equation. The external forces are balanced by the tension of the elastic spring. Thus

$$-\tau u_{xx} = f(x)$$

for $0 < x < 1$ and $u(0) = u(1) = 0$.

3 Deformation of an Elastica

The transverse deformation of a thin elastic in extensional rod subjected to an axial loading and clamped at its ends is governed by the differential system;

$$\frac{d^2\theta}{ds^2} + P\sin\theta = 0,$$
$$0 < s < 1, \theta(0) = \theta(1) = 0$$

.

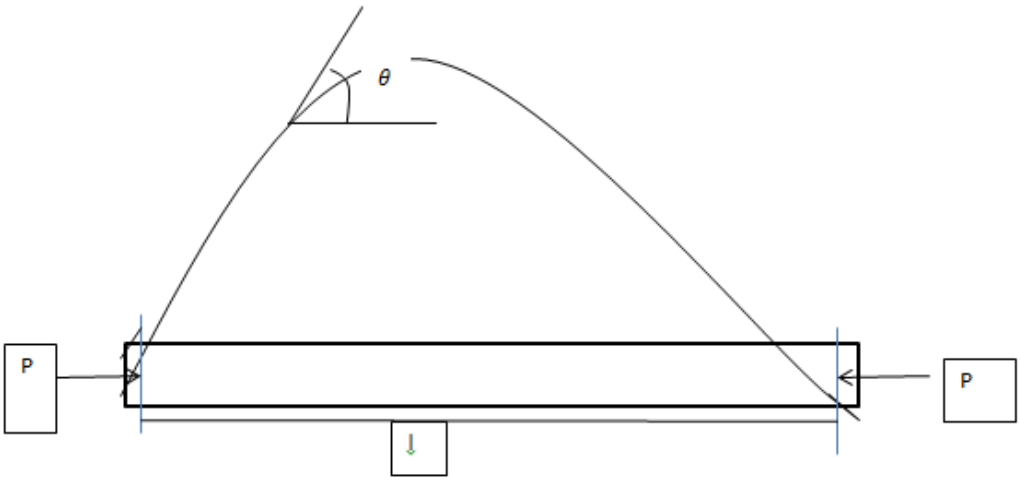

Figure 1.1: Elastic deformation

The figure (1.1.2) shows the rod with unit length, magnitude of the loading equal to P, and θ is the angle that the deformed rod makes with the initial undeformed axis. This classical second-order non-linear

two-point boundary value problem is called the elastic problem. The solution, however becomes unstable as P increases and the rod bends into a deformed shape. Hence, this boundary value problem is also a differential eigenvalue problem that consists of determining θ and the critical load P for deformed shapes to exist. Once θ has been determined the Cartesian co-ordinates of a deformed point on the rod can be determined as the solution of the initial value problems.

An example of physical phenomena occurs in Boggio - Hadamard conjecture for a clamped plate. Given that $u(x)$ denotes the deviation from the equilibrium of the idealised one dimensional beam at point x, then

$$u''(x) = f$$

where

$$u(x_0) = u(x_n) = 0$$

1.2 Background of the problem

The laws of nature can be fashioned in the language of differential equations namely partial differential equations, PDE and ordinary differential equations, ODE. Just like many physical phenomena, the Schrodinger's Equation, SE can be described as a PDE for the time dependent, and ODE when considering the time independent SE. The S.E. plays the role of second Newton's law and conservation of energy in classical mechanics i.e. it predicts the future behaviour of a dynamic system. It is closely related to the second Newton's law of motion $F = ma$.

According to quantum mechanics, we describe systems using wave functions. It incorporates duality of matter ,that is, a system can act as a wave or particle. Thus a system such as that of an electron can be described by using the wave function. For example, in this case, the wave may represent the displacement or amplitude of the wave produced by that electron in space. If we treat the system as a particle, then the wave function is used to give us the probability of finding the particle at some point$|\phi|^2$. In order to describe any system in quantum mechanics, we must be able to determine what the wave function is numerically. In quantum mechanics, the Schrodinger's equation describes how the quantum state of a physical system changes with

time. It is therefore the fundamental equation of the non-relativistic quantum mechanics which involves ODEs of second order in which the first order does not occur explicitly. The study of this equation plays an exceptionally important role in modern physics. It was formulated in late 1925 and published in 1926, by the Austrian Physicist Erwin Schrodinger.

The concept of a wave function is a fundamental postulate of quantum mechanics. For standard interpretation of quantum mechanics, the wave function is the most complete description that can be given of a physical system. Schrodinger's equation describes not only molecular, atomic and subatomic systems but also macroscopic systems even for the whole universe.

In the past other methods have been used to solve this equation including perturbation theory, variational method and density functional.

Use of numerical schemes in solving the Schrodinger's equation has also been on the rise. Iterative and finite difference methods that converge to a solution faster and do not require a lot of storage are preferred. Thus there has been a need to obtain efficient solution for solution of the time independent Schrodinger's equation which in this study is by use of Lobtto quadrature method.

1.3 Statement Of The Problem

This involves the study of the numerical solution of ordinary differential equations in solving time independent Schrodinger's equation. Since the solutions to be obtained and their efficiency will help other readers to comprehend how the solution of this equation has been done over the years and also to use the most efficient numerical methods.

1.4 Objective of the study

The purpose is to investigate an efficient numerical scheme to the time independent Schrodinger's equation.

1.5 Specific Objectives

1. To study the numerical solution for ordinary differential equations used in solving Schrodinger's equation.

2. To find the energy eigenvalues and the corresponding eigenfunctions for the Woods- Saxon potential using a sixth order numerical scheme.

3. To check the accuracy by comparing with the analytic solution for a Woods-Saxon potential with the computed value.

CHAPTER 2

LITERATURE REVIEW

Boundary value methods based on either collation or finite differences are not very popular for the solution of time independent Schrodinger's equation, TISE due to the fact that the problem is based on the infinite interval.

Initially, the Schrodinger's equation used to be solved with a guessed energy, that always made the wave function to blow up at the infinity. Thus trial and error was used to find an energy for which the wave function is tamed up to a very large value of the radius.

An alternative approach for developing efficient methods, for the solution of TISE is to use exponential fitting curves. Raptis and and Allison (1981) in [2] had derived Numerov's type exponentially fitted method.

Vanden et al (1989) in [19] investigated the numerical methods for solving radial Schrodinger's equation of the type

$$\left(\frac{d^2}{dr^2} - F(E,r)\right) U(r) = 0$$

where

$$F(E,r) = \frac{l(l+1)}{r^2} - (E - V(r))$$

Rieth and Schommers (2002) in [34] developed a novel numerical method

for the solution of Schrodinger's Equation for a particle in an interaction potential of the general shape. This method for the quantum-mechanical determination of the eigenstates and eigenvalues of a particle (e.g. an electron) in a potential of general shape. For such, the method allows to calculate the exact solutions of the stationary Schrodinger's Equation. A transition from the stationary reference system to the stationary system under investigation is performed by means of the TISE. The results are thus compared with various alternative numerical methods.

Maike Schulte (2007) in [35] solved the Schrodinger's equation numerically on an unbounded domains i.e. $r \to 0$ and $r \to \infty$. Here he discussed and analysed the results on open boundary conditions for the two-dimensional time-dependent Schrodinger's Equation. The aim was to derive new mathematical models for the simulation of novel electronic devices of nano-scale dimensions. It thus derives a new dicretisation scheme of the two dimensional Schrodinger's equation.

Tatu et al (2007) in [13] solved the eigenvalue problem for the Schrodinger's equation using Numerov's method which is so far the highest ordered method and at the same time a three-point method. Lower order methods such as fourth order Runge- Kutta method leads to smaller net intervals, h and hence longer integration times and more round off errors.

The current research realised that methods involving more than three adjacent functions values should be avoided, since they are frequently unstable. It therefore studied the Numerov's theory for integrating the one- dimensional time independent Schrodinger's equations.

$$y'' = f(x)y(x), f(x) = V(x) - E, x \in [a, b]$$

with non-singular potential V(x). Numerov's method of order 4 is superior to other methods since besides having the same phase-lag order as the four-step methods it has also a larger interval of periodicity. It also requires less starting values.However its rate of convergence is slower.

Thus the current study is meant to highlight on the previous methods which have been used in the past and to contribute to the missing link on a method which leads to a faster rate of convergence. Hence the use of sixth order numerical scheme derived using Lobatto Quadrature, also known as Radau Quadrature.

CHAPTER 3

SCHRODINGER'S EQUATION AND ITS NUMERICAL SCHEMES

3.1 Overview of Schrodinger's Equation

The Schrodinger equation plays the role of Newton's law and conservation of energy in classical mechanics i.e. it predicts the future behaviour of a dynamic system. It is a wave equation in terms of the wave function which predicts analytically and precisely the probability of events or outcome. The detailed outcome is not a large number of events, the Schrodinger equation, S.E. will predict the distribution results.

Total energy in terms sum of kinetic energy and potential energy, $\frac{1}{2}mv^2 + \frac{1}{2}kx^2$, are transformed into Hamiltonian which acts upon the wave function to generate the evolution of the wave function in the space. The Schrodinger's equation gives the quantized energies of the system. The SE exists in both time dependent (partial differential equation) and time independent forms (ordinary differential equation) forms.

The S.E. is both an inter-twin of both quantum mechanics and the wave function, ϕ. Quantum mechanics was motivated by two kinds of experimental observations; quantisation energy transfer in light-matter interactions, and

the dual wave- particle of both light and matter. Thus motivated, Max Planck to correctly calculate the spectrum of the black -body radiation in 1900 by postulating that an electromagnetic field can exchange energy with atoms only in quanta which are the product of the radiation frequency and the constant h; i.e.

$$E = hf \tag{3.1}$$

3.2 Derivation of Schrodinger's Equation

This is done by first stating some useful results from previous authors which are also utilised in the derivation of the Schrodinger's equation.

1. Albert Einsten's Result

$$E = hf_0 + \frac{1}{2}mv^2 = W_0 + \frac{p^2}{2m} \tag{3.2}$$

where h is Plank's constant, f_0 is the threshold frequency v, the velocity, p the momentum of the wave particle and W_0 is the work function.

2. Niel's Result

$$h = \frac{\hbar}{2\pi} \tag{3.3}$$

3. Bor's and de Broglie's Results

$$p = \frac{h}{\pi} \tag{3.4}$$

where p is the momentum of wave particle.

Erwin Schrdinger was motivated by de Broglie's ideas and set his mind on finding a wave equation for the electron. He used Maxwell's equations for electromagnetic fields. The wave equation governing electromagnetic waves in free space is derived from Maxwell's equation in free space, which are;

$$\nabla XE = -\frac{\partial B}{\partial t} \tag{3.5}$$

$$\nabla XB = \frac{1}{c^2}\frac{\partial E}{\partial t} \tag{3.6}$$

$$\nabla .E = 0 \tag{3.7}$$

$$\nabla .B = 0 \tag{3.8}$$

where **c** is the speed of light in vacuum, **E** is the electric field and **B** is the magnetic field. The equations (3.5), (3.6), (3.7), (3.8) are referred to as Faraday's law, Ampere's law, Gauss law for electricity and Gauss law for magnetism respectively.

Schrodinger's equation has been derived by several physicists but this describes derivation by Schrodinger himself where he began with the classical wave equation, as derived by Maxwell's equations governing electrodynamics.

The Maxwell's first law given by equation (3.5) illustrates generation of a voltage by a changing magnetic field (electromagnetic induction) which is the basis of functioning of generators, inductors and transformers. The second law given by equation (3.6) embodies Ampere's law and is the magnetic equivalence of the first equation. It explains why there is a circulating magnetic field surrounding a wave with electrical current running through it as used in the electromagnetic and magnetic poles associated with the rotating ion core in the earth. The third law given by equation (3.7) stipulates that charge is a source for the electric field. If charges are present, then the right-hand side of equation (3.7) is non-zero and proportional to the charge density. The equation (3.8) is the magnetic case which can be referred to as "no magnetic monopoles"law.

Applying the curl operator to both sides of equation (3.5), and substituting $\nabla X B$ from equation (3.6), yields

$$\nabla X(\nabla X E) = -\frac{1}{c^2}\frac{\partial^2 E}{\partial^2 t} \tag{3.9}$$

Let $\vec{V}$ be any vector; using the following vector identity

$$\nabla X(\nabla X\vec{V}) = \nabla X((\nabla.\vec{V}) - \nabla^2 V)$$

Applying this to the left hand side of equation (3.9) yields

$$\nabla X(\nabla X E) = \nabla(\nabla.E) - \nabla^2 E$$

Using equation (3.7), this reduces to

$$\nabla^2 E = -\frac{1}{c^2}\frac{\partial^2}{\partial t^2} = 0$$

which is the electromagnetic wave equation. It can be written as

$$\frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = 0 \tag{3.10}$$

Solving equation (3.10) by method of separation of variables for example, let the solution of (3.10) be

$$E(x,t) = \psi(x)T(t) \tag{3.11}$$

The equation 3.10 is satisfied by the plane wave equation.

$$E(x,t) = E_0 e^{i(kx-\omega)t} \tag{3.12}$$

where $K = \frac{2\pi}{\lambda}$ and $\omega = \pi f$ in which K and f are the spatial and temporal frequencies respectively, which must satisfy the dispersion relation obtained upon substitution of (3.12) into (3.10)

$$\Rightarrow \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial^2 t}\right) E_0 e^{i(kx-\omega t)} = 0$$

$$\Rightarrow \left(-k^2 + \frac{\omega^2}{c^2}\right) E_0 e^{i(kx-\omega t)} = 0$$

Solving the wave vector, we arrive at the dispersion relation for light in the free space:

$$k = \frac{\omega}{c} \tag{3.13}$$

or $c = f\lambda$ relation represents classical electromagnetic waves and is related to the theory of quantum photons.
From Einsten, that energy of a photon is

$$\begin{aligned} E - hf &= \hbar\omega \\ \hbar &= \frac{h}{2\pi} \\ \omega &= 2\pi f \end{aligned}$$

where ω is the angular velocity and the momentum of a photon is

$$p = \frac{h}{\alpha} = \hbar K$$

Thus (3.12) can be written as

$$E(x,t) = E_0 e^{(px-\varepsilon t)}$$

Substituting into (3.10), we obtain

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) - E_0 e^{(px-\varepsilon t)} = 0 \tag{3.14}$$

$$-\frac{i}{\hbar^2}\left(p^2 - \frac{\varepsilon^2}{c^2}\right) E_0 e^{\frac{i}{\hbar}(px-\varepsilon t)} = 0 \tag{3.15}$$

$$\varepsilon^2 = p^2 c^2 \tag{3.16}$$

The relativistic total energy, is thus given by $\varepsilon^2 = p^2c^2 + m^2c^4$ for a particle with zero rest mass, which is right since light is made of photons.

Next, assuming with de Broglie that frequency and energy and wavelength and momentum, are related in the same way for classical particles as for photons, and consider a wave equation for non-zero rest, mass particles. Thus getting $\varepsilon^2 = p^2c^2 + m^2c^4$ instead of $\varepsilon^2 = p^2c^2$. Since there is no dealing with electric field, we can give the solution to our wave equation a new name say ψ and call it a wave function. This shows that (3.14) is homogeneous and hence the units of the function operated upon are arbitrary. Equation (3.15), now becomes;

$$\frac{1}{\hbar^2}\left(p^2 - \frac{\varepsilon^2}{c^2} + m^2c^2\right)\psi e^{\frac{i}{\hbar}(px-\varepsilon t)} = 0 \tag{3.17}$$

can be obtained from

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\psi e^{\frac{i}{\hbar}(px-\varepsilon t)} = 0 \tag{3.18}$$

Since light is treated as a collection of photons, the square of the electric field is proportional to the number of photons. Thus our wave function

$$\psi(x,t) = \psi_0 e^{\frac{i}{\hbar}(px-\varepsilon t)} \tag{3.19}$$

can be normalised to a unit probability. Then, the probability. Then, the probability that the particle is located somewhere in space is;

$$\int_{-\infty}^{\infty} \psi.\psi = 1 \tag{3.20}$$

Removing restriction to one dimension and rearranging, we obtain this as the Klein- Gordon equation for a free particle,

$$\nabla^2\psi - \frac{m^2c^2}{\hbar^2}\psi = \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} \tag{3.21}$$

Klein - Gordon is a relativistic equation hence Schrodinger had to take necessary assumptions to establish a non- relativistic equation.

The first step is to approximate $\varepsilon^2 = p^2c^2m^2c^4$ as follows;

$$\varepsilon = mc^2\sqrt{1 + \frac{p^2}{m^2c^2}} \tag{3.22}$$

$$\approx mc^2\left(1 + \frac{1}{2}\frac{p^2}{m^2c^2}\right) \tag{3.23}$$

$$\approx mc^2 + \frac{p^2}{2m} = m^2 + T \tag{3.24}$$

The last term is the classical Kinetic energy ,T. Thus equation (3.19) can be rewritten as

$$\psi(x,t) = \psi_o e^{\frac{i}{\hbar}(px - mct - Tt)} \tag{3.25}$$

$$e^{\frac{-i}{\hbar}(mc^2t)}\psi_0 e^{\frac{i}{\hbar}(px - Tt)} \tag{3.26}$$

Assuming that the particle velocity is small such that $mv << mc$, which implies that $p^2 << m^2c^2$. Thus the leading term in equation (3.26) , $e^{\left(\frac{-imc^2t}{\hbar}\right)}$ will oscillate much faster than the last term, $e^{\left(\frac{iTt}{\hbar}\right)}$. Thus

$$\psi = e^{\frac{-i}{\hbar}mc^2t}\phi \tag{3.27}$$

where

$$\boldsymbol{\psi} = \phi_0 e^{\frac{i}{\hbar}(px-Tt)} \tag{3.28}$$

Then

$$\frac{\partial\psi}{\partial t} = \frac{-i}{\hbar}mc^2 e^{\frac{-i}{\hbar}(mc^2t)}\phi + e^{\frac{-i}{\hbar}(mc^2t)}\frac{\partial\phi}{\partial t} \tag{3.29}$$

$$\frac{\partial^2\psi}{\partial t^2} = \left(\frac{-m^2c^2}{\hbar^2}e^{\frac{-i}{\hbar}(mc^2t)}\phi - \frac{2i}{\hbar}mc^2 e^{\frac{-i}{\hbar}mc^2t}\frac{\partial\phi}{\partial t}\right) \tag{3.30}$$

Discarding the last term since it is small and approximating in equation (3.18), we get

$$e^{\frac{-i}{\hbar}mc^2t}\left[\frac{\partial^2}{\partial x^2} + \frac{2im}{\hbar}\frac{\partial}{\partial t}\right]\phi = 0 \tag{3.31}$$

$$\frac{\partial^2\phi}{\partial x^2} + \frac{2im}{\hbar}\frac{\partial\phi}{\partial t} = 0 \tag{3.32}$$

Rearranging and generalising to three spatial dimensions, we finally arrive at the Schrodinger's equation

$$\frac{-\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + V(x)\phi(x,t) = i\hbar\frac{\partial\phi}{\partial t} \tag{3.33}$$

which is called the Schrodinger's time dependent equation, TDSE, and where the non-relativistic wave function ϕ is also constrained to the condition that it be normalizable to unit probability. In one dimension when $t = 0$, the equation (3.33) reduces to time independent Schrodinger's equation, (TISE) which is an ordinary oifferential equation and is written as;

$$\frac{-\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) = E\phi(x) \tag{3.34}$$

where V(x) is the local potential difference and $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$ is the K.E. operator. In equation (3.34) , the left hand side is the Hamiltonian operator of the wave function.

The TISE predicts that wave functions can form standing waves called stationary state, and the general solution is given by

$$\phi(x) = \phi(x)e^{\frac{-iEx}{\hbar}} \tag{3.35}$$

For N particles, in one dimension the Hamiltonian is;

$$\hat{H} = \sum_{n=1}^{N} \frac{\hat{p}^2}{2M_n} + V(x_1, x_2, \ldots, x_N), \hat{p}_n^2 = -i\hbar\frac{d}{dx_n}$$

where the position of particle n is x_n. The corresponding TISE is

$$\frac{-\hbar^2}{2}\sum_{n=1}^{N}\frac{1}{m_n}\frac{d^2\phi(x_1, x_2, \ldots, x_N)}{dx^2} + V(x_1, x_2, \ldots, x_N)\phi(x_1, x_2, \ldots, x_N) = E\phi(x_1, x_2, \ldots, x_N)$$

and hence the general solution takes the form

$$\phi(x_1, x_2, \ldots, x_N) = e^{\frac{-iE}{\hbar}}\phi(x_1, x_2, \ldots, x_N)$$

For non-interacting distinguishable particles, the potential of the system only influences each particle separately, so that the total potential energy is the sum of the potential energies for each particle:

$$V(x_1, x_2, \ldots, x_N) = \sum_{n=1}^{N} V(x_n)$$

and the wave function can be written as a product of the wave functions for each particle:

$$\phi(x_1, x_2, \ldots, x_N) = \Pi_{n=1}^{N}\phi(x_n)$$

For the bound states, the boundary conditions is that the wave function goes to zero as $x \to \pm\infty$ i.e. picking a finite value of $|x| = a$ and assuming that

wave functions are identically zero at those values of x to generate the two-point boundary value problem i.e.

$$\frac{-\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x = E\phi(x)$$

and

$$\phi(-a) = \phi(a) = 0$$

3.3 Methods for solving Time-Independent Schrodinger's Equation

3.3.1 Matrix diagonalisation method

The one dimensional Schrodinger's equation may be written as;

$$\left[\frac{d^2}{dx^2} - f(x)\right] y(x) = 0, f(x) = u(x) - E, \tag{3.36}$$

where $u(x) = \left(\frac{2m}{\hbar^2}\right) V(x), E = \left(\frac{2m}{\hbar^2}\right) \varepsilon$ and u(x) and E represents the potential and the energy in dimensionless form. For the purpose of numerical treatment, we write it as;

$$y'' + [E - u(x)]y = 0 \tag{3.37}$$

where;

$$E\phi = \frac{-\hbar^2}{2m}\frac{d^2\phi}{\dot{\mathrm{x}}^2} + V(\vec{r})\phi \tag{3.38}$$

If the potential is independent of x, then the solution to this equation can be written as;

$$\phi(x,t) = AE^{-\frac{iEt}{\hbar}+iKx} \tag{3.39}$$

$$\phi(x = 0) = \phi(x = L) = 0 \tag{3.40}$$

This method aims at transforming the given differential equation to matrix equation.

First set up a lattice of discrete points and record the value of the function at each lattice point (nodes). The corresponding value for each lattice point is a value for the wave function.
Then, $\phi(x_n)$ generates a column vector indicating its values at different ϕ points.

$$\phi(x) = \begin{bmatrix} \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_n) \\ \vdots \\ \phi(x_N) \end{bmatrix}$$

Then $E\phi = -\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + U(\vec{r})\phi$

$$\Rightarrow E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} H \\ N \times N \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

The eigenvalues of $N \times N$ of H therefore be evaluated. This produces N eigenvalues and N eigenvectors.

Thus $[V, D] = eig(H)$ where D has the eigenvalues of matrix H as its diagonal elements, V has normalized eigenvectors of H as its columns.
Considering the case of a particle in a box;

$$E\phi = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\phi$$

Consider $E\phi = [V(x)]\phi$ since $V(x)$ is a potential function on a discrete lattice V would tell us the potential at each lattice point, hence it will be diagonal.

$$E\phi_n = V(x_n)\phi_n \Rightarrow E \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix} = \begin{bmatrix} H = V(x) \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{bmatrix}$$

and

$$V(x) = \begin{bmatrix} V_1 & 0 & 0 & \dots & 0 \\ 0 & V_2 & 0 & \dots & 0 \\ 0 & 0 & V_3 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \\ 0 & 0 & 0 & \dots & V(x_N) \end{bmatrix}$$

But E is given by

$$E\phi = \frac{-\hbar^2}{2m}\frac{d^2\phi}{dx^2}$$

Rewriting $\dfrac{d^2\phi}{dx^2}$ in terms of central difference operator beginning with;

$$\left[\frac{d\phi}{dx}\right] : \left[\frac{d\phi}{dx}\right]_{n+\frac{1}{2}} = \frac{\phi_n + 1 - \phi_n}{h}$$

and

$$\left[\frac{d\phi}{dx}\right]_{n-\frac{1}{2}} = \frac{\phi_n - \phi_n - 1}{h}$$

hence

$$\left[\frac{d^2\phi}{dx^2}\right]_n = \left[[\frac{d\phi}{dx}]_{n+1/2} - [\frac{d\phi}{dx}]_{n-1/2}\right]/h$$

$$\Rightarrow \frac{\phi_{n+1} - 2\phi_n + \phi_{n-1}}{h^2} \Rightarrow E\phi_n = t_0[2\phi_n - \phi_{n+1} - \phi_{n-1}]$$

where $t_0 = \dfrac{\hbar^2}{2mh^2}$

$$\Rightarrow E\begin{bmatrix}\phi_1\\ \phi_2\\ .\\ .\\ .\\ \phi_N\end{bmatrix} = t_0\begin{bmatrix}2 & -1 & 0 & 0 & 0 & 0\\ -1 & 2 & -1 & 0 & 0 & 0\\ 0 & -1 & . & . & & \\ 0 & 0 & . & . & & \\ 0 & 0 & . & . & & \\ 0 & 0 & . & . & . & -1\\ 0 & 0 & . & . & -1 & 2\end{bmatrix}\begin{bmatrix}\phi_1\\ \phi_2\\ .\\ .\\ \phi_n\\ .\\ \phi_N\end{bmatrix}$$

which is a tridiagonal matrix. Inclusion of the potential matrix yields

$$E\phi_n = U(x_n) - t_o(\phi_{n-} - 2\phi_n + \phi_{n+1})$$

Hence

$$E\begin{bmatrix}\phi_1\\ \phi_2\\ .\\ .\\ \phi_n\\ .\\ \phi_N\end{bmatrix} = \begin{bmatrix}2t_0 + U(x_1) & -t_0 & 0 & 0 & 0 & 0\\ -t_0 & 2t_0 + U(x_2) & -t_0 & 0 & 0 & 0\\ 0 & -t_0 & . & & & \\ 0 & 0 & . & . & & \\ 0 & 0 & . & . & & \\ 0 & 0 & . & . & & -t_0\\ 0 & 0 & . & . & -t_0 & 2t_0 + U(x_N)\end{bmatrix}\begin{bmatrix}\phi_1\\ \phi_2\\ .\\ .\\ \phi_n\\ .\\ \phi_N\end{bmatrix}$$

3.3.2 Runge - Kutta of order 4

This is used in the solution of

$$\frac{d^2y}{dx^2} = \alpha f(x, y) = 0 \tag{3.41}$$

where $y(a) = \beta y(b) = \gamma$, is a constant. β and γ are constants and are the values of the function, y at the both boundaries. Equation (3.41) is reduced to two first ordinary differential equations by assuming

$$\frac{dy}{dx} = p = f_{n1}(x, y, p) \tag{3.42}$$

then

$$\frac{dp}{dx} = -\alpha f_{n2}(x, y, p) \tag{3.43}$$

The solution y(x) for this problem from $x_0 = a$ to $x_n = b$ where the step length h is given by;

$$h = \frac{x_n - x_o}{n}$$

The set of 1st order ODEs 3.42 and 3.43 are solved together from the following formula.

$$\left.\begin{aligned} y_{n+1} &= y_n + \tfrac{1}{6}(K_1 + 2K_2 + 2K_3 + K_4) \\ p_{n+1} &= p_n + \tfrac{1}{6}(L_1 + 2L_2 + L_3 + L_4) \end{aligned}\right\} \tag{3.44}$$

where $K_1, K_2, K_3, K_4, L_1, L_2, L_3 and L_4$ are calculated as follows:

$$\left.\begin{aligned} K_1 &= hf_{n1}(x_n, y_n, p_n) \\ L_1 &= hf_{n2}(x_n, y_n, p_n) \\ K_2 &= hf_{n1}(x_n + \tfrac{h}{2}, y_n + \tfrac{K_1}{2}, p_n + \tfrac{L_1}{2}) \\ L_2 &= hf_{n2}(x_n + \tfrac{h}{2}, y_n + \tfrac{K_1}{2}, p_n + \tfrac{L_1}{2}) \\ K_3 &= hf_{n1}(x_n + \tfrac{h}{2}, y_n + \tfrac{K_2}{2}, p_n + \tfrac{L_2}{2}) \\ L_3 &= hf_{n2}(x_n + \tfrac{h}{2}, y_n + \tfrac{K_2}{2}, p_n + \tfrac{L_2}{2}) \\ K_4 &= hf_{n1}(x_{n+h}, y_n + K_3 + p_n + L_3) \\ L_4 &= hf_{n2}(x_{n+h}, y_n + K_3 + p_n + L_3) \end{aligned}\right\} \tag{3.45}$$

3.3.3 Runge Kutta Butcher of 6th order method

The BVPs of second order is solved by RBK of 6th order. Applying this method to solve equations 3.42 and 3.43 by the formula given

$$\left.\begin{aligned} y_{n+1} &= y_n + \tfrac{h}{90}(7K_1 + 32K_2 + 12K_4 + 32K_5 + 7K_6) \\ p_{n+1} &= p_n + \tfrac{h}{90}(7L_1 + 32L_2 + 12L_4 + 32L_5 + 7L_6) \end{aligned}\right\} \tag{3.46}$$

where the constants $K_1, K_2K_3, K_4, K_5, K_6, L_1, L_2, L_3, L_4, L_5$ and L_6 are calculated as follows;

$$\left.\begin{aligned}
&K_1 = f_{n1}(x_n, y_n, p_n)\\
&L_1 = f_{n2}(x_n, y_n, p_n)\\
&K_2 = f_{n1}(x_n, y_n, p_n) + \tfrac{h}{4}L_1\\
&L_2 = f_{n2}(x_n + \tfrac{h}{4}, y_n + \tfrac{hK_1}{4}, p_n + \tfrac{hL_1}{4})\\
&K_3 = f_{n1}(x_n, y_n, p_n) + \tfrac{hL_1}{8} + \tfrac{hL_2}{8}\\
&L_3 = f_{n2}(x_n + \tfrac{h}{4}, y_n + \tfrac{hK_1}{8} + \tfrac{hK_2}{8}, p_n + \tfrac{hL_1}{8} + \tfrac{hL_2}{8})\\
&K_4 = f_{n1}(x_n, y_n, p_n) - \tfrac{hL_2}{2} + hL_3\\
&L_4 = f_{n2}(x_n + \tfrac{h}{2}, y_n - \tfrac{hK_2}{2} + hK_3, p_n - \tfrac{hL_2}{2} + hL_3)\\
&K_5 = f_{n1}(x_n, y_n, p_n) + \tfrac{3hL_1}{16} + \frac{9L_4}{16}\\
&L_5 = f_{n2}(x_n + \tfrac{3h}{4}, y_n + \tfrac{3hK_1}{16} + \frac{9hK_4}{16}, p_n - \tfrac{3hL_1}{16} + \frac{9hL_4}{16})\\
&K_6 = f_{n1}(x_n, y_n, p_n) - \tfrac{h}{7}(3L_1 - 2L_2 - 12L_3 + 12L_4 - 8L_5)\\
&L_6 = f_{n2}[x_n + h, y_n - \tfrac{h}{7}(3K_1 - 2K_2 - 12K_3 + 12K_4 - 8K_5)\\
&, p_n - \frac{h}{7}(3L_1 - 2L_2 - 12L_3 + L_4 - 8L_5)]
\end{aligned}\right\} \quad (3.47)$$

p_0 is predicted from

$$p_r^{(0)} = \left[\frac{y^{(1)} - y^{(0)}]}{h}\right]$$

then $p(0)$ is modified by

$$p_{(0)}^{r+1} = p_{(0)}^{r} + \left(\frac{(y_{(1)}^{r} - y_{(1)}}{h}\right)$$

3.3.4 Numerov's Method

The time independent Schrodinger's equation can be written in a more general way as

$$y'' = f(r, y) \quad (3.48)$$

This can be solved by deriving difference equations corresponding to equation 3.48or tansforming it into a system of first order equations or by means of Numerov's method with uniform partition of the finite interval$(0, \vec{r})$;

$$0 = r_0 < r_1 < r_2 < \ldots < r_n = \bar{r}, r_k = kh$$

where $k = 0, 1, 2, ..., n$

Using Taylor's theorem under the assumption that f and $y(r)$ are sufficiently smooth, we write

$$y(r_i + h) = y(r_i + 1) = y(r_i) + hy'(r_i) + \frac{h^2}{2!}y''(r_i) + \ldots \tag{3.49}$$

Replacing h by $-h$ in equation (3.49) entails

$$y(r_i - h) + y(r_i) - hy'(r_i)\frac{h^2}{2!}y''(r_i) + \ldots \tag{3.50}$$

Combining equations (3.49) and (3.50) yields

$$y(r_i + h) - 2y(r_i) + y(r_i - h) = \frac{2h^2}{2!}y''(r_i)y''(r_i) + \frac{2h^4}{4!}y^{(4)}(r_i) + \ldots \tag{3.51}$$

which when differentiated twice yields the following equation

$$y''(r_i + 1) - 2y''(r_i) + y''(r_i - 1) = \frac{2h^2}{2!}y^{(4)}(r_i) + \frac{2h^4}{4!}y^{(6)}(r_i) + \ldots \tag{3.52}$$

from equation 3.51

$$h^2y^{(4)}(r_i) = y''(r_i + 1) - 2y''(r_i) + y''(r_i - 1) - \frac{2h^4}{4!}y^{(6)}(r_i) + \ldots \tag{3.53}$$

and this equation yields in turn, with the use of equation (3.53) in equation (3.51)

$$\begin{aligned} &y(r_i + 1) - 2y(r_i) + y(r_i - 1) = h^2y''(r_i) + \frac{h^2}{12}[\frac{1}{h^2}[y''(r_i + 1)- \\ &2y''(r_i) + y''(r_i - 1)\frac{2h^4}{12!}y^{(6)}(r_i) + \ldots]] + \frac{2h^6}{6!}y(6)(r_i) \\ &= \frac{h^2}{12}\left[y''(r_i + 1) + 10y''(r_i) + y''(r_i - 1)\right] - \frac{3h^6}{6!}y^{(6)}(r_i) + O(h^8) \end{aligned} \tag{3.54}$$

Substituting by means of equation (3.48) and eliminating the 6th order terms in equation (3.54) gives us the Numerov's method of order four, which is two step method. It is an implicit method and is reducible to an explicit equation whenever f is linear in y as is the case with Schrodinger's equation.

3.3.5 Method of De Vogelaere

This method has flexibility in allowing changes in stepsize during the integration. Consider equidistant points $x_0 = a, x_1, x_2, \ldots, x_{2n} = b$ with mesh spacing$h$. At each integration k $(k = 0, 1, 2, \ldots, n-1)$ the De Vogelaere's algorithm consists of three formulas which compute (in the stated order) $[\bar{y}_{2k+1}, \bar{y}_{2k+2}, \bar{y'}_{2k+2}]$ in terms of the given $[\bar{y}_{2k-1}, \bar{y}_{2k}, \bar{y'}_{2k}]$

An upper bound for the local truncation error is established, the interval of absolute stability is [-2,0] and it is shown that its global truncation error is of order h where h is the step length. Consider equidistant points $x_0 = a, x_1, x_2, \ldots, x_2 n = b$ with mesh spacing h. It is important to note that the odd and even-labelled points play distinct rules since the last point for the computation must be even-labelled points play distinct rules since the last point for the computation must be even-labelled. At each iteration $k(k = 0, 1, 2, \ldots, n-1)$ the De Vogelaere algorithm consists of three formulae which compute (in the stated order) $[\bar{y}_{2k+1}, \bar{y}_{2k+2}, \bar{y'}_{2k+2}]$ in terms of given $[\bar{y}_{2k-1}, \bar{y}_{2k}, \bar{y'}_{2k}]$ Using Taylor's theorem to expand $y(x)$ and $f(x) = f(x, y(x))$ about the point x_{2k} we obtain;

$$y(x_{2k} + \lambda) = y(x_{2k}) + \lambda y'(x_{2k}) + \frac{\lambda^2}{2!} y''(x_{2k}) + \ldots + \frac{\lambda^p}{p!} y^p(x_{2k}) + \ldots \quad (3.55)$$

$$f(x_{2k} + \lambda) = f(x_{2k} + \lambda f'(x_{2k} + \frac{\lambda^2}{2!} f''(x_{2k}) + \ldots + \frac{\lambda^p}{p!} f^p(x_{2k}) + \ldots \quad (3.56)$$

where

$$y''(x) = f(x), y'''(x) = f'(x), y^{(4)} = f''(x) + \ldots$$

The first expression is given by;

$$I_1 = \frac{h^2}{6}[4f(x_{2k}) - f(x)_{2k-1}],$$

which is transformed to a form of order h^5. On using equation (3.56) with $\lambda = -h$, we have

$$\left.\begin{aligned}
&\frac{h^2}{6}\left[4f(x_{2k}) - f(x_{2k-1})\right] \\
&= \frac{h^2}{6}\left[4f(x_{2k}) - f(x_{2k}) - hf'(x_{2k}) + \frac{h^2}{2}f''(x_{2k}) + O(h^3)\right] \\
&= \frac{h^2}{6}\left[3f(x_{2k}) + hf'(x_{2k}) - \frac{h^2}{2}f''(x_{2k})\right] + O(h^5) \\
&= \frac{h^2}{2!}f(x_{2k}) + \frac{h^3}{3!}f'(x_{2k}) + \frac{h^4}{4!}f''(x_{2k}) - (\frac{1}{12} + \frac{1}{4!})h^4 f''(x_{2k}) + O(h^5) \\
&= \frac{h^2}{2!}y''(x_{2k}) + \frac{h^3}{3!}y'''(x_{2k}) + \frac{h^4}{4!}y^{(4)}(x_{2k}) - \frac{1}{8}h^4 f''(x_{2k}) + O(h^5) \\
&= y(x_{2k+1}) - y(x_2k) - hy'(x_{2k}) - \frac{1}{8}h^4 f''(x_{2k}) + O(h^5)
\end{aligned}\right\} \tag{3.57}$$

where the first and last terms give

$$y(x_{2k+1}) = y(x_{2k}) + hy'(x_{2k}) + \frac{h^2}{6}[4f(x_{2k}) - f(x_{2k_1})] + \frac{1}{8}h^4 f''(x_{2k}) + O(h^5) \tag{3.58}$$

The second expression is

$$I_2 = \frac{h^2}{3}[4f(x_{2k+1}) + 2f(x_{2k})]$$

setting $\lambda = h$ in equation (3.56) and retaining terms upto order h^6 gives;

$$\left.\begin{aligned}
&\frac{h^2}{3}[4f(x_{2k+1}) + 2f(x_{2k})] \\
&= \frac{h^2}{3}\left[4f(x_{2k}) + hf'(x_{2k}) + \frac{h^2}{2}f''(x_{2k}) + \frac{h^3}{6}f'''(x_{2k}) + O(h^4) + 2f(x_{2k})\right] \\
&= \frac{h^2}{3}\left[6f(x_{2k}) + 4hf'(x_{2k}) + 2h^2 f''(x_{2k}) + \frac{(2h)^3}{3}f'''(x_{2k})\right] O(h^6) \\
&= 2\frac{(2h)^2}{2!}f(x_{2k}) + \frac{(2h)^3}{3!}f'(x_{2k}) + \frac{(2h)^4}{4!}f''(x_{2k}) + \frac{(2h)^5}{5!}f'''(x_{2k}) + \frac{2}{9} - \frac{2^5}{5!}
\end{aligned}\right\} \tag{3.59}$$

Thus

$$h^5 f'''(x_2 x) + O(h^6) = y(x_{2k+2}) - y(x_{2k}) - 2hy'(x_{2k}) - \frac{2}{45}h^5 f'''(x_{2k}) + O(h^6)$$

from which we solve for;

$$y(x_{2k+2}) = y(x_{2k}) + 2hy'(x_{2k}) + \frac{h^2}{3}\left[4(f_{2k+1}) + f(x_{2k})\right] + \frac{2}{45}h^5 f'''(x_{2k}) + O(h^6) \tag{3.60}$$

The remaining third term expression to be calaculated is

$$I_3 = \frac{h}{3}[f(x_{2k}) + 4f(x_{2k+1}) + f(x_{2k+2})]$$

and evaluate this upto terms of $O(h^6)$, namely

$$\left.\begin{array}{l} \frac{h}{3}[f(x_{2k}) + f(x_{2k+1}) + f(x_{2k+2})] \\ = \frac{h}{3}[f(x_{2k}) + 4[f(x_{2k}) + hf'(x_{2k}) + \frac{h^2}{2!}f''(x_{2k}) + \frac{h^3}{3!}f'''(x_{2k}) \\ + \frac{h^4}{4!}f^{(4)}(x_{2k}) + O(h^5)] + f(x_{2k}) + 2hf'(x_{2k}) + \frac{(2h)^2}{2!}f''(x_{2k}) + \\ \frac{(2h)^3}{3!}f'''(x_{2k}) + \frac{(2h)^4}{4!}f^{(4)}(x_{2k}) + 0(h^5)] \\ = 2hf(x_{2k}) + \frac{(2h)^2}{2!}f'(x_{2k}) + \frac{(2h)^3}{3!}f''(x_{2k}) + \frac{(2h)^4}{4!}f'''(x_{2k}) + \\ \frac{(2h)^5}{5!}f^{(4)}(x_{2k})) + (\frac{5}{18}\frac{2^5}{5!})h^5 f^{(4)}(x_{2k}) + 0(h^6) \\ = 2hy''(x_{2k}) + \frac{(2h)^2}{2!}y'''(x_{2k}) + \frac{(2h)^3}{3!}y^{(4)}(x_{2k}) + \frac{(2h)^4}{4!}y^{(5)}(x_{2k}) + \\ \frac{(2h)^5}{5!}y^{(6)}(x_{2k}) + \frac{1}{90}h^5 f^{(4)}(x_{2k}) + O(h^6) \end{array}\right\} \tag{3.61}$$

so that

$$y'(x_{2k+2}) = y'_(x_{2k}) + \frac{h}{3}f(x_{2k}) + 4f(x_{2k+1}) + f(x_{2k+2}) - \frac{1}{90}h^3 f^{(4)}(x_{2k}) + O(h)^6 \tag{3.62}$$

The De Vogelaere algorithm consists of the three formulas equations (3.58), (3.60) and (3.62) wherein terms of order h^4, h^5, and h^6 are neglected, therefore, the algorithm is as follows;

Given $(\bar{y}_{2k-1}, \bar{y}_{2k}, \bar{y}'_{2k})$ compute first

$$f_{2k} = f(x_{2k}, \bar{y}_{2k})$$

,

$$f(x_{2k-1} = f(x_{2k-1}, \bar{y}_{2k-1})$$

,and thereafter

$$(\bar{y}'_{2k+1})$$

from

$$\bar{y}'_{2k+1} = \bar{y}'_{2k} + h\bar{y}'_{2k} + \frac{h^2}{6}[4f_{2k} - f_{2k-1}], \tag{3.63}$$

Compute second

$$f_{2k+1} = f(x_{2k+1}, \bar{y}_{2k+1})$$

and thereafter $\bar{y}_{2k+2}$ from

$$\bar{y}'_{2k+2} = \bar{y}'_{2k} + 2h\bar{y}'_{2k} + \frac{h^2}{3}[4f_{2k+1} + 2f_{2k}], \tag{3.64}$$

and compute the third one $f_{2k+2} = f(x_{2k+2}, \bar{y}_{2k+2})$ and thereafter $\bar{y}'_{2k+2}$ from

$$\bar{y}'_{2k+2} = \bar{y}_{2k} + \frac{h}{3}[f_{2k} + 4f_{2k+1} + f_{2k+2}] \tag{3.65}$$

The derivatives at the odd-labelled mesh points are absent in this algorithm. The even labelled points are more accurate than those at odd-labelled ones.

The local truncation errors in y_{2k+2} and y'_{2k+2} are of order 5 while that of y_{2k+1} is of order 4. It is not self starting hence to overcome this,

$$y_{-1} = y_0 - z_0 + \frac{h^2}{2}f_0$$

where f_{-1} is calculated and has an error term of order h^3.

If $y(x)$ is the exact solution of the initial-value problem, the global truncation errors in the function and derivative values at the end of the n^{th} De Volelaere step are

$$y(x_{2n-1} - y_{2n-1}) = e_n^{(1)}, \tag{3.66}$$

$$y(x_{2n} - y_{2n}) = e_n^{(2)}, \tag{3.67}$$

$$y'(x_{2n} - y'_{2n}) = \frac{e_n^{(3)}}{h} \tag{3.68}$$

$$\tag{3.69}$$

3.3.6 Piecewise Pertubation Methods

The given equation is replaced by another differential equation (called reference equation), which can be solved exactly. Perturbation theory estimates the deviation of the solution of the reference equation from the original equation.

Each piecewise perturbation method is defined by the recipe used for the piecewise approximation of the coefficients of the differential equation considered: if then the method is referred to as a *constant* perturbation method, whereas if they are approximated by piecewise lines, then it is called a line perturbation method.
Piecewise Pertubation approach is used to solve equations of the kind

$$y'' = f(x)y(x)$$

with $x \in [a, b]$ where $f(x)$ is some bounded real function. Introducing a partition of [a,b]: $x_0 = a < x_1 < x_2 <, \ldots < x_n = b$. There is no special restriction upon the manner of distributing the mesh points except if $f(x)$ is discontinuous at one point, then such a point should be taken as a mesh point. We concentrate on the piecewise pertubation algorithm which propagate the solution from x_k all the way up to x_{k+1}
Introducing the variable $\sigma \in [0, h_k]$ and denote $X = x_k$ and $g(\delta) = f(X + \delta)$ then the one step problem is

$$y''(X + \delta) + g(\delta)y(X + \delta) \tag{3.70}$$

CHAPTER 4

APPLICATION OF LOBATTO QUADRATURE

4.1 TISE and Woods-Saxon Potential

A basic problem in the nuclear physics is the motion of the free electrons which have a conclusive influence on the abundance of metallic clusters. These electrons are moving in well defined orbitals, around the central nucleus and in a mean field potential which is produced by the positively charged ions and the rest of the electrons. In the mean field potential, the details of the potential are described by free parameters such as depth , width and the slope of the potential, which have to be fitted to experimental observation. Thus a mean field potential is always empirical and its an example given by the Woods-Saxon potential. The TISE is given by

$$\frac{d^2\phi}{dx^2} = [V(x) - E(x)]\phi(x) \tag{4.1}$$

subject to $\phi(0) = 0$ for $x \to \pm\infty$. E is a real number denoting the energy value and V is a given function which denotes the potential. E is the eigenvalue while ϕ is the eigenvector of the Schrodinger's equation. The value of V is dicretised depending on how it occurs.

The potential V(x) is given by;

$$V(x) = \frac{pp}{c(x)} + \frac{Q}{c^2(x)} \exp\left(\frac{x - x_0}{a_0}\right) \tag{4.2}$$

where $c(x) = 1 + exp\left(\frac{x - x_0}{a_0}\right)$ and PP, Q, a_0 and x_0 are numerical parameters. The Woods-Saxon potential is much used in nuclear physics. Solving numerically for the eigenvalues. The following choice of parameters. $x_0 = 7$, $a_0 = 0.6$, $pp = -50$, $Q = \frac{pp}{a_0}$ as agreed upon by Adams et al [18]. u_0 is the potential depth, while x_0 is width of the potential and a_0 its diffuseness and is the surface thickness which is usually adjusted to the experimental values of ionization energies. Substitution of the parameters into The Woods-Saxon potential yields

$$V(x) = \frac{-50}{1 + exp[(x-7)/0.6]} + \frac{Q}{(1 + exp[(x-7)/0.6])^2} \exp\left(\frac{x-7}{0.6}\right) \tag{4.3}$$

4.2 Derivation of the sixth order scheme using Lobatto quadrature

It also called Radau quadrature method. It a Gaussian quadrature method with the weighting function$W(x)1$ in which the endpoints of the interval [-1, 1] are include in a total of n nodes thus resulting in $r = n - 2$ .The general formula is

$$\int_{-1}^{1} f(x)dx = W_1 f(-1) + W_n f(1) + \sum_{i=2}^{n} W_i f(x_i)$$

The free abscissas x_i for $i = 2, \ldots, n-1$ are the roots of the polynomial, $P'_{n-1}(x)$, where $P(x)$ is a Legendre polynomial. The weights are obtained by:

$$W_i = \frac{2n}{[1 - x_i^2]P''_{n-1}(x_i)P'_m(x_i)}$$

$$= \frac{2}{n(n-1)[P_{n-1}(x_i)]^2}$$

and the end points are given by

$$W_{1,n} = \frac{2}{n(n-1)}$$

and the error term is given by

$$E = -\frac{n(n-1)^3 2^{2n-1}[(n-2)!]^4}{(2n-1)[(2n-2)!]^3} f^{2n-2}(\xi)$$

for $\xi \in (-1, 1)$. The coefficients of W_i are positive. The algebraic degree of accuracy is $2n-2$. There exists tables of nodes and Weights for the Lobatto quadrature in [22]

4.2.1 Generating a sixth numerical scheme Lobatto quadrature formula

Given $y'' = F(x, y)$ where $x \in [a, b]$ with $R_1(y) = \gamma_1$ and $R_2(y) = \gamma_2$ such that $h = \left(\frac{b-a}{n}\right)$ with y_n denoting the approximation to the value at $y(x)$ at $x = x_n$

$$\delta^2 y(x_n) = \int_{x_n}^{x_{n+1}} (x_{n+1} - t)[y''(t) + y''(2x_n - t)]dt \tag{4.4}$$

Using

$$t = x_n + \frac{h}{2}(1 + u)$$

Then Integrating by parts and letting

$$u = x_{n+1} - t$$

and

$$dv = y''(t) + y''(2x_n - t)$$

and using change of variables; then we obtain

$$\delta^2 y(x_n) = y(x_{n+1}) - 2y(x_n) + y(x_{n-1}$$

and

$$\delta^2 y(x_n) = \int_{x_n}^{x^{n+1}} (x_{n+1} - t)[y''(t) + y''(2x_n - t)]dt$$

$$\delta^2 y(x_n) = \frac{h^2}{4}\int_{-1}^{1}(1-u)[y''(x_n - \frac{h}{2}(1+u)) + y''(x_n + \frac{h}{2}(1+u))]du$$

Evaluating this by a known quadrature formula; the weighting function in the integral can be taken as 1 or $1-u$. Or rewrite the integral using the expression

$$w_0 y''(x_n) + w_1[y''(x_{n-1}) + y''(x_{n+1})]\sum_{i=1}^{p} W_{r_i}[y''(x_n - r_i h) + y''(x_n + r_i h)] + E \tag{4.5}$$

where w_0, w_1 and w_{r_i} are the weights and r_i are the abscissas and E is the truncation error.

$$\delta^2 y_n = h^2[w_0 y''_n + w_1(y_{n-1} + y''_{n+1}) + \sum_{i=1}^{p} w_{r_i}(y''_{n-r_i} + y''_{n+r_i})] \tag{4.6}$$

Taking $p = 3$ and expanding both sides of equation (4.6) in a Taylor's series about $x = x_n$ and equate the coefficients of the powers of h up to six. This will generate a sixth order scheme. We get 3 equations in eight unknowns. The w_i are solved in terms of the $r_i's$, which are chosen as the abscissas of the quadrature formula or as the values which optimize the order of the difference scheme. The values of $y(x)$ at $x = x_{n\pm r_i}$ are not known. This can be done an by approximating using a fifth order approximation to $y_{n\pm r_i}$ as follows;

$$y_{n+q} = (1-q)y_n + qy_{n+1} + \frac{q(q-1)}{24}h^2[(q^2-q-1)y''_{n-1}$$

$$-2(q^2+q-5)y''_n + (q^2+3q+3)y''_{n+1}] + T_n^*$$

$$y_{n-q} = (1-q)y_n + qy_{n-1} + \frac{q(q-1)}{24}h^2[(q^2+3q+3)y''_{n-1} - 2(q^2+q-5)y''_n$$

$$+(q^2-q-5)y''_n + (q^2-q-1)y''_{n+1}] + T_n^{*'}$$

where $q = r_i, i = 1, 2, 3$ and

$$T_n^* = \frac{1}{360}(3q^5 - 10q^3 + 7q)h^5 y^{(5)}(x_n) + \frac{1}{1440}[2q^6 - 5q^4 + 3]h^6 y^{(6)}(\xi_3) \quad (4.7)$$

$$T^{*'} = -\frac{1}{360}(3q^5 - 10q^3 + 7q)h^5 y^{(5)}(x_n) + \frac{1}{1440}[2q^6 - 5q^4 + 3q]h^6 y^{(6)}(\xi_4) \quad (4.8)$$

where $x_n < \xi_3, \xi_4 < x_{n+1}$ Based on Lobatto integration, the finite difference scheme becomes;

$$\delta^2 y_n = \frac{h^2}{12}[2y_n'' + 5s(y_{n-r}'' + y_{n+r}'') + 5r(y_{n+s}'')] \quad (4.9)$$

where $r = \left(\frac{5-\sqrt{5}}{10}\right)$ and $s = \left(\frac{5+\sqrt{5}}{10}\right)$. Using this scheme to solve the schrodinger's equation subject to $y(a) = y(b) = 0$, we use the second approximation scheme in [32] to determine the values of $y_{n\pm r}$ and $y_{n\pm s}$ and put them in equation (4.9) and obtain

$$(-1 + A_n)y_{n-1} + (2 + B_n)y_n + (-1 + C_n)y_{n+1} = D_n \quad (4.10)$$

for $n = 1, 2, 3, \ldots, N - 1$
This can be simplified as

$$My = (J + Q)y = B$$

where M is $N - 1$ matrix is the sum of J and Q matrices which form a tridiagonal matrix where the non-zero elements are given by $j_{i,i} = 2$, and $j_{i+1,i} = -1$ and $q_{i,i} = B_i, q_{i+1,i} = A_i, qi, i + 1 = C_i$ and $B = (b_i)$ is and $(n - 1)$- dimensional column vector such that

$$b_1 = D_1, b_i = D_i, i = 2, 3, 4, \ldots, N - 2$$

$$b_{N-1} = D_{N-1}$$

The values of A_n, B_n, C_n and D_n for the approximation are given as in [32]

4.2.2 Sixth order Lobatto quadrature method for solution of TISE

The TISE is given by equation (3.34) and can be rearranged to give:

$$\frac{h^2}{2m}\frac{d^2\phi(x)}{dx^2} = V(x)\phi(x) - E\phi(x) \quad (4.11)$$

but experimentally the ratio of $\hbar^2 : 2m$ has been found to be one. Thus we have

$$\frac{d^2\phi(x)}{dx^2} = V(x)\phi(x) - E\phi(x) = f(x)\phi(x) \tag{4.12}$$

where

$$f(x) = [e - V(x)]$$

and

$$\phi''(x) = \frac{\phi(x-h) - 2\phi(x) + \phi(x+h)}{h^2}$$

but $\mathbf{H}\phi = E\phi$ where the square matrix $\mathbf{H}$ is the Hamiltonian operator of the system and it is equal to the sum of the Kinetic energy and potential energy. The eigenvectors of $\mathbf{H}$ are the stationary states of the time-independent Schrodinger equation and the eigenvalues are the corresponding energies of the Stationary states.

During calculations, fix the minimum amount of energy say E_{min} say -50 (for this study) and maximum energy, E_{max} to be 1010. The negative energies leads to abound state problemcondition. The minimum local de Broglie wavelength is given by

$$\lambda = \frac{\hbar}{\sqrt{E_m}} \tag{4.13}$$

Grid spacing h corresponding to about one point per radian i.e. $h = \lambda/2\pi$. The number of grid points needed can be estimated by finding the outer turning points x_t such that $V(x_t) = E_m$ and allowing for an extra 2λ into classically forbidden region.

Thus N can be determined by the formula $N = (\frac{2x_t}{h} + 4\pi)$ rounded to the nearest energy. If N is first fixed, the $x_t = (N/2 - 4\pi)h$ which simplifies to

$$x_t = (\frac{(N/2 - 4\pi)}{\sqrt{E_M}})$$

Numerov's scheme is thus used to find the energy at different states after putting a trial energy for the initial energy. The found energy is thus iterated up to required degree of accuracy. Considering the minimum energy to be negative energy yields a bound state problem with the boundary conditions given as:

$$y(0) = 0$$

and

$$y(x) = \exp(-\sqrt{-E})$$

for large values of x. During the numerical treatment, the values of energy values are computed in the internal points only for different bound states.

This can be solved using Woods- Saxon potential and the results obtained. Inthe solution, the variables are changed such that we replace $\delta^2 y(x)$ by $\delta^2\phi$ in equation (4.9) and obtain equation (4.14)

$$\phi_{i-1} - 2\phi_i + \phi_{i+1} = \frac{h^2}{12}\left[2f_i\phi_i + 5s(f_{i-r}\phi_{i-r} + f_{i+1}\phi_{i+1}) + 5r(f_{i+s}\phi i + s)\right] \tag{4.14}$$

Where

$$\begin{aligned} f_i &= -E + V_i \\ f_{i-r} &= -E + V_{i-r} \\ f_{i+r} &= -E + V_{i+r} \\ f_{i+s} &= -E + V_{i+s} \end{aligned}$$

Solution of this equation yields the energy values as shown in the results shown in the tables (5.1), (5.2), (5.3) and (5.4) respectively for various values of the step length h.

CHAPTER 5

RESULTS AND DISCUSSIONS

5.1 Results

The results in table (5.1) to (5.4) show the values of the various bound state energies with their corresponding errors when different values of step lengths (indicated) are used in computation.

Table 5.1: **Woods-Saxon Potential using Numerov's and the Sixth order scheme with** $h = \frac{1}{4}$

Energy states	Exact Values	E_{val} by Sixth order	Errors From Nume	Errors in Sixth order
E_1	-49.457788728	-49.45778874	0.3598×10^{-4}	0.1248×10^{-7}
E_2	-48.148430420	-48.14843007	0.6811×10^{-4}	0.3515×10^{-6}
E_3	-46.290753954	-46.29075974	0.6889×10^{-3}	0.5789×10^{-5}
E_4	-43.968318432	-43.96834815	0.2690×10^{-2}	0.2972×10^{-4}
E_5	-41.236077720	-41.23637122	$0.4583 \times 10^{-}2$	0.2935×10^{-3}
E_6	-38.122785097	-38.1317581	0.1998×10^{-1}	0.8973×10^{-2}

Table 5.2: **Woods-Saxon Potential using Numerov's and the Sixth order scheme $h = \frac{1}{8}$**

Energy states	Exact Values	E_{val} by Sixth order	Errors From Nume	Errors in Sixth order
E_1	-49.457788728	-49.45778874	0.3598×10^{-4}	0.1248×10^{-7}
E_2	-48.148430420	-48.14843065	0.5396×10^{-3}	0.2174×10^{-6}
E_3	-46.290753954	-46.29075721	0.7857×10^{-4}	0.3251×10^{-5}
E_4	-43.968318432	-43.96831947	0.1264×10^{-3}	0.1036×10^{-5}
E_5	-41.236077720	-41.23616744	$0.2984 \times 10^{-}3$	0.8972×10^{-4}
E_6	-38.122785097	-38.123368	0.1177×10^{-2}	0.6517×10^{-3}

Table 5.3: **Woods-Saxon Potential using Numerov's and the Sixth order scheme $h = \frac{1}{16}$**

Energy states	Exact Values	E_{val} by Sixth order	Errors From Numerov's	Errors in Sixth order
E_1	-49.457788728	-49.45778874	0.3598×10^{-4}	0.1248×10^{-7}
E_2	-48.148430420	-48.14843051	0.5396×10^{-4}	0.9261×10^{-7}
E_3	-46.290753954	-46.1484305	0.4350×10^{-4}	0.7561×10^{-7}
E_4	-43.968318432	-43.968319	0.4322×10^{-5}	0.5691×10^{-6}
E_5	-41.236077720	-41.2364434	$0.3473 \times 10^{-}2$	0.3657×10^{-3}
E_6	-38.122785097	-38.12283621	0.7867×10^{-4}	0.5111×10^{-4}

Table 5.4: **Woods-Saxon Potential using Numerov's and the Sixth order scheme** $h = \frac{1}{32}$

Energy states	Exact Values	E_{val} by Sixth order	Errors From Nume	Errors in Sixth order
E_1	-49.457788728	-49.45778874	0.3598×10^{-4}	0.1248×10^{-7}
E_2	-48.148430420	-48.14843048	0.5396×10^{-4}	0.6293×10^{-7}
E_3	-46.290753954	-46.29075399	$0.4350 \times 10^{-}4$	0.3572×10^{-7}
E_4	-43.968318432	-43.96833095	0.4322×10^{-5}	0.1252×10^{-4}
E_5	-41.236077720	-41.23608291	$0.3473 \times 10^{-}2$	0.5192×10^{-5}
E_6	-38.122785097	-38.12279303	0.4340×10^{-3}	0.7932×10^{-5}

5.2 Discussion

During calculations of the ground state energy, the trial energies that give not solutions are inserted and the output difference is only minimised at the ground state for various energy levels. The solution is calculated for some energy E_0. The technical part is how to choose this energy so that the eigenvalues lies inside the required interval above which it can cause ionisation effect. Bound states energy solutions of the TISE exists only for discrete eigenvalues.

The calculations are improved beginning with the trial energies E which should be chosen within the allowed band. i.e. below an eigenstate, ϕ_{left} and ϕ_{right} are computed for the $E + \Delta E$ where ΔE is some energy increment. The difference changes sign. Once a sign change occurs, then the $\Delta E = -\frac{\Delta E}{2}$ and repeated until the desired accuracy is obtained.

The computed value is then compared with the analytical value. The interest is to find the eigenvalue of the each bound state using a Lobatto quadrature method.

The numerical results indicate that the new method is much more accurate than the Numerov's method. We conclude that finite difference schemes offers an easy way to solve the 1D Schrodinger's equation numerically. Generally, the results are more accurate for higher order finite difference methods. For example, for the Woods-Saxon Potential problem, we obtained more accurate results with a small number of grid points .

By comparing the output for the analytical solutions of the non-dimensional

Schrodinger's equations, it can be verified that the sixth order numerical scheme gave sufficiently accurate results. In summary, the sixth order method is efficient in determining the eigenstates and eigenvalues of a particle in generally shaped interaction potentials. It is evident from the various tables that decreasing the size of the step length reduces the magnitude of the error. Thus higher accuracy is obtained when computations for the same number of iterations are done for relatively smaller values of step lengths.

If a microscopic system is conservative, then there is a quantum states of the system, called stationary states, in which the energy is sharper at the bound states.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

This research was based on investigating the numerical solution of one dimensional time independent Schrodinger's equation using the sixth order Lobatto quadrature method. This was achieved and the results compared against those obtained by Numerov's method. The results implies that the sixth order method yields smaller errors as compared to that of Numerov's method. In addition, smaller step lengths significantly leads to reduced magnitude of errors. The current study also highlights on various methods which have also been used in past to solve the same equation.

6.2 Recommendations

In the findings of this study, I recommend the following:

✓The choice of the higher value of energy should be done well otherwise the computed energies will diverge from the analytic solution for high quantum numbers.

✓Possible extension to this work in finding more efficient numerical schemes of higher orders to compute the bound state energies for the same boundary conditions.

✓This research can be extended to finding energy values for higher bound states with care taken on choice of minimum energy to avoid ionisation of the electrons involved.

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