SOLOMON MATHEW KARMA, A DISECTION OF BESSEL FUNCTIONS AND APPLICATIONS TO SOLUTION OF SCHRÖDINGER TIME INDEPENDENT EQUATION IN CYLINDRICAL AND SPHERICAL WELL. NEU, 2017

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A THESIS SUBMITTED TO THE GRADUATE SCHOOL OF APPLIED SCIENCES OF NEAR EAST UNIVERSITY

By

SOLOMON MATHEW KARMA

In Partial Fulfillment of the Requirements for the Degree of Master of Science in Mathematics

NICOSIA, 2017

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Approval of Director of Graduate School of Applied Sciences

Prof. Dr. Nadire Cavus.

We certify that, this thesis is satisfactory for the award of the degree of Master of Sciences in Mathematics.

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I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I have fully cited and referenced all materials that are not original work of this thesis.

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Date:

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To those who believe in me…

ABSTRACT

This thesis is meant to examine the study of Bessel functions, their properties and applications, as they relate to solutions of Schrödinger time independent equation, in accordance with their polar coordinates. Bessel functions in general have vast applications in practical life situations and posses interesting properties, which make them, served as basic tools for studying applied science like mathematical physics and engineering. Due to interest and time constraint, we shall dissect the Laplace equation in each coordinates of cylindrical and spherical system, in order to uncover some special types of differential equation, whose solution are obtain to be those of Bessel functions in each of the coordinates, via the Frobenius method of series solutions. We shall show that these solutions relates with those of Schrödinger time independent equation of a zero and infinite potentials in cylindrical and spherical well.

The properties and behaviours of these solutions are further examine together with their boundary conditions to reveal the usefulness of zeros of Bessel functions, in order to normalized the solutions of these special type of differential equation and to show that the energy of the systems can easily be computed separately.

Furthermore the numerical solution of estimated errors, of the first and second order accuracy difference schemes was calculated.

Keywords: Cylindrical well; Spherical well; Schrödinger equation; Bessel functions; Laplace equation.

ÖZET

Bu tez, kutupsal koordinatlarına göre Schrödinger zaman bağımsız denkleminin çözümleriyle ilgili oldukları Bessel fonksiyonlarının incelenmesi, özellikleri ve uygulamaları incelenecektir. Bessel fonksiyonlarının genel olarak pratik yaşam koşullarında geniş uygulamaları vardır ve ilginç özelliklere sahiptir ve bunları matematiksel fizik ve mühendislik gibi uygulamalı bilim eğitimi için temel araç olarak kullanırlar. Faiz ve zaman kısıtlaması nedeniyle çözümü, koordinatların her birinde Bessel fonksiyonlarının elde ettiği bazı özel diferansiyel denklem tiplerini ortaya çıkarmak için, silindirik ve küresel sistemin her bir koordinatında Laplace denklemini inceleyeceğiz. Seri çözümlerin Frobenius yöntemi. Bu çözümlerin, sıfır ve sonsuz potansiyellerin Schrödinger zamandan bağımsız denklemiyle silikon ve küresel olarak iyi ilişkili olduğunu göstereceğiz.

Bu çözümlerin özellikleri ve davranışları, bu özel tip diferansiyel denklemlerin çözümlerinin normalleştirilmesi ve sistemlerin enerjisinin kolayca bulunabileceğini göstermek için sınır koşullarıyla birlikte Bessel fonksiyonlarının sıfırlarının kullanışlılığını ortaya koymak için birlikte incelenir Ayrı olarak hesaplanmıştır.

Ayrıca, birinci ve ikinci dereceden doğruluk farkı düzenlerinin tahmini hatalarının sayısal çözümü hesaplanmıştır.

Anahtar Kelimeler: Silindirik kuyu; Küresel kuyu; Schrödinger denklemi; Bessel fonksiyonları; Laplace denklemi.

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LIST OF SYMBOLS

$\boldsymbol{\psi}(\mathbf{r},\mathbf{t})$: Wave function.

$\mathbf{V}(\mathbf{r},\mathbf{t})$: Potential energy.

$\mathbf{m}$: Mass of particle/body.

$\boldsymbol{\nabla}$: Laplace symbol.

$\boldsymbol{\hbar}$: Planck constant.

$\mathbf{J_k}(\mathbf{z})$: Bessel functions of first kind integer order.

$\mathbf{Y_k}(\mathbf{z})$: Bessel functions of second (Neumann function) integer order.

$\mathbf{H_k^{(1)}}(\mathbf{z})$: Hankel Bessel functions of first kind integer order.

$\mathbf{H_k^{(2)}}(\mathbf{z})$: Hankel Bessel functions of second kind integer order.

$\mathbf{I_k}(\mathbf{z})$: Modified Bessel functions of first kind integer order.

$\mathbf{K_k}(\mathbf{z})$: Modified Bessel functions of second kind integer order.

$\mathbf{g}(\mathbf{z},\mathbf{x})$: Generating function.

$\mathbf{j}_{\boldsymbol{\ell}}(\mathbf{kr})/\mathbf{j_p}(\mathbf{t})$: Spherical Bessel functions of first kind.

$\mathbf{n}_{\boldsymbol{\ell}}(\mathbf{kr})/\mathbf{n_p}(\mathbf{t})$**:** Spherical Bessel functions of second kind (Neumann function).

$\mathbf{h_p^{(1)}}(\mathbf{z})$: Spherical Hankel Bessel functions of first kind.

$\mathbf{H_p^{(2)}}(\mathbf{z})$: Spherical Hankel Bessel functions of second kind.

$\mathbf{P_x}$: Momentum of a body/particle.

E: Energy of the system.

A: Amplitude.

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CHAPTER ONE
INTRODUCTION

In this section we present the background of our study, present a brief literature on the topic, highlight the problem and analyze some definitions and theorems as they relates to the topic.

The concept of Bessel's function was first presented by Euler, Lagrange and Bernoulli in 1732. Daniel Bernoulli made the first to attempt to use Bessel's function of zero order, as a solution to examine the situation of an oscillating chain hanging at one end. However, Leonard Euler in 1764 also used Bessel's function of zero order and integral order to analyze the vibration in a stretched membrane. The work was re-investigated and modified by Lord Rayleigh in 1878, where he defined Bessel's solution to be a special case arising from Laplace wave equation.

Although Bessel's functions are named after Friedrich .W. Bessel, in 1839, he did not explored the concept until in 1817, where he uses them as a solution of Kepler problem, to examined the mutual gravity of three bodies moving in motion. In 1824 he later presented Bessel's functions as the solution to a planetary perturbation problem, which appears to be a sort of expansion of coefficient of series of a direct perturbation planet, where the movement of the sun is caused by the perturbation of the particle.

The notation $J_n(z)$ were first used to denotes Bessel's functions, (Hansan, 1843). Schlomilch, (1857) also adopted the same notation to denote Bessel's functions. The notations $J_n(z)$ were later modified to $J_n(2z)$ (Watson, 1922).

Bessel functions are found to appear in practical problems of real situation and are extensively investigated by many scholars in many diverse applications to a real life situation, where they surface more frequently. For instance Bessel functions surface in practical applications such as in electricity, hydrodynamics and diffraction (Yasar and Ozarslan, 2016).

However Bessel's equations and Bessel's functions are uncovered to be solution of problems that occur from solving the Laplace equation and Helmholtz equation in polar coordinate system (i.e. in cylindrical symmetry and spherical symmetry), (Watson, 1922). They are also discovered when solving some problem in physics for instance, the aging spring problem, heavy chain problem, the lengthen pendulum problem e.tc, by employing a suitable change of variable to transforme these equations into a special kind of equation called the Bessel's differential equations and there after obtain special types of solution known to be Bessel functions.

Bessel's functions are found to be some special kind of functions that have vast applications in sciences and engineering. For instance, they occurred in the study of heat conduction, oscillations problems, vibrations problems and electrostatics potential (Yasar and Ozarslan,2016). Basically, when problems are solved in the cylindrical coordinates the solutions obtained are found to be Bessel's functions of integer order, which occurred in many practical problems of real situations, while problems that are handled at spherical coordinate systems are found to be Bessel functions of half or semi integer order. The spherical Bessel's function can also be presented in form of trigonometric function, due to the behavior of the series solution obtained. The Bessel spherical function of semi integer order, have vast application in mathematical physics for instance, in quantum mechanics, they revealed the solution of radial Schrödinger equation of particle with zero potentials, scattering of electromagnetic radiation, frequency dependent friction, dynamical systems of floating bodies e.tc (Yasar and Ozarslan,2016).

Erwin Schrödinger in 1926, in a bit to examine the De-Broglie hypothesis, uncovered an equation, which in a way exhibits same properties, with that of the particle of an electron. Although the equation uncovered, was later named after him as Schrödinger equation and was presented in Laplace equation form as

$$\left(-\frac{\hbar}{2m}\nabla^2 + V(r,t)\right)\psi(r,t) = i\hbar(r,t), \tag{1.1}$$

where m is defined as the mass of the particle/body, $V(r,t)$ as the potential energy, and $\psi(r,t)$ as the wave function of the particle, (Griffith, 1995).

The electromagnetic wave equation and some basic properties of Einstein's theory like relativity plays a central idea in understanding the nature and concept of Schrödinger equation, has it stands now, Schrödinger equation is the most remarkable and essential equation in the studies of modern physics, because of its vast applications. Equation (1.1) is described as the Schrödinger time dependent equation, from which the Schrödinger time independent equation is derived. For the purpose of this thesis, the Schrödinger time independent equation for a free particle shall be our reference point, which we shall derive later.

However, this thesis is meant to study the Bessel functions, their properties and applications, as they relate to solution of Schrödinger equation in polar coordinates. Bessel functions in general have large applications in real situations and posses interesting properties, which make them, served as basic tools for studying natural sciences like mathematical physics and engineering. Due to interest and time constraint, we shall dissect the Laplace equation in their in two polar coordinates of cylindrical and spherical systems, in order to uncover some special types of differential equation, whose solution are those of Bessel functions in two seperate coordinates, obtained via the Frobenius method of series solutions, we shall show that these solutions are those of Schrödinger equation of a free particle in both cylindrical and spherical well.

The properties and nature of these solutions are further examine together with their boundary conditions to reveal the usefulness of zeros of Bessel functions, in order to normalize the solutions of these special type of differential equation and to compute the energy of this systems.

In our work, we shall consider one problem, which will be examined in their respective coordinates of cylindrical and spherical systems.

The problem is as follows: Suppose we place a particle of mass m, in a two dimensional potential well, with zero and infinite radius, inside and outside the box respectively, (Griffith, 1995).

Their respective Laplace equation is represented in their polar coordinates as

$$\nabla^2\psi(r,\phi) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi(r,\phi)}{\partial r}\right) + + \frac{1}{r^2}\frac{\partial^2\psi(r,\phi)}{\partial\phi^2} \tag{1.2}$$

Similarly,

$$\nabla^2 F = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\left(\frac{\partial^2 f}{\partial\emptyset^2}\right) \tag{1.3}$$

In our work, we shall examine equations (1.2) and (1.3), in their respective coordinates, by employing mathematical method of separating their variables to suit the nature of their solution. Furthermore, we wish to examine the above equations together with the problem stated above, in their respective coordinates, in order to analyze the nature of the solution when the boundary conditions are applied to their general solutions and uncover the uniqueness of zeros of Bessel functions in the entire process.

1.1 Some Fundamental Definitions

Definition 1.1.1 Convergence, Zill, (2005).

The power series of the form $\sum_{n=0}^{\infty}(z - z_0)^n$, converges at a finite value of z, when the partial sum $(s_n(z))$ converges. Implying,

$\lim_{n\to\infty} s_n(z) = \sum_{n=0}^{\infty}(z - z_0)^n$, exist. Otherwise, the series diverged.

Definition 1.1.2 Analytic function, Arnold, (2005).

At a point z_0, a function f is analytic, when a series of the form $y(z) = \sum_{n=0}^{\infty}(z - z_0)^n$, converges for all point of z, in the interval containing z_0.

Definition 1.1.3 Differential Equation of Order Two, Zill, (2005).

Given the a differential equation of the form,

$$\mathbf{a_2(z)\frac{d^2y}{dz^2} + a_1(z)\frac{dy}{dz} + a_0(z)y} \qquad \mathbf{(1.4)}$$

where $a_2(z)$, $a_1(z)$, and $a_0(z)$ are function of z and we can express equation (1.4), in another form as

$$\frac{d^2y}{dz^2} + P(z)\frac{dy}{dz} + Q(z)y = 0 \qquad (1.5)$$

Where $P(z) = \frac{a_1(z)}{a_2(z)}$ and $Q(z) = \frac{a_0(z)}{a_2(z)}$

1.1.4 Ordinary and Singular Point: Zill, (2005).

If P(z) and Q(z) in equation (1.4) are differentiable and continuous at a point z_0, then z_0 , is an ordinary point, else a point which is not an ordinary point, is a singular point of equation (1.5).

1.1.5 Regular and Irregular Point: Zill, (2005).

If $p(z) = (z - z_0)P(z)$ and $q(z) = (z - z_0)^2Q(z)$ are differentiable and continuous at z_0 , then z_0 , is a regular singular point of equation (1.4) , else an irregular point z_0.

1.1.6 Recurrence formulae: Borelli and Coleman, (1998).

A recurrence formulae for coefficients of c_n, is a relation for which each c_n is evaluated in terms of $c_0, c_1, c_2, \ldots, c_{n-1}$; if the differential equation in equation (1.4), is evaluated then such formulae can be obtain and is express in terms of power series at $z = z_0$.

1.1.7 Gamma Function: Brenson, (1973).

For any positive real number p, let denote $\Gamma(p)$ to be gamma function, then we have

$$\Gamma(p) = \int_0^\infty z^{p-1} e^{-z} dz \tag{1.6}$$

Thus, the equation of gamma function is

$$\Gamma(p+1) = p\Gamma(p)$$

It is important to note that factorial function (which is given for nonnegative integers) is a general case of gamma function. We can write factorial as $\Gamma(n+1) = n!$

For example: $\Gamma(p+2) = (p+1)\Gamma(p+1), \Gamma(p+3) = (p+2)\Gamma(p+2)$

$$= (p+2)(p+1)\Gamma(p+1)$$

1.2 Some Important Theorems

1.2.1 Frobenius' Theorem: Zill, (2005).

Suppose in equation (1.4), $z = z_0$ is a regular singular point, then at least one solution exist in the form

$$y(z) = (z - z_0)^\partial \sum_{n=0}^\infty c_n (z - z_0)^n = \sum_{n=0}^\infty c_n (z - z_0)^{n+\partial} \tag{1.7}$$

where n and ∂ , are the indexes and ∂ is to be computed as the roots of the series. Thus, the series will converge around the region of $0 < |z - z_0| < R$.

1.2.2 Power Series Existence: Simmon, (1972).

In equation (1.5), if the ordinary point is $z = z_0$, then the series with centre at z_0, is linearly independent. i.e.

$$y(z) = \sum_{n=0}^\infty c_n (z - z_0)^n,$$

where, at the interval $|z - z_0| < R$ the series solution converges, implying that R is the distance from z_0 to the closest singular point.

Theorem 1.2.3: Zill, (2005).

Suppose in equation (1.4), z_0 is a regular singular point, where ∂_1 and ∂_2 are the roots of equation (1.4), at z_0. Note that both ∂_1 and ∂_2, are real, then

Case I: suppose that $\partial_1 - \partial_2 = 0$ then two linearly independent solutions of equation (1.4), exists in the form

$$\begin{cases} y_1(z) = \sum_{n=0}^{\infty} c_n (z - z_0)^{n+\partial_1} \\ y_2(z) = \sum_{n=0}^{\infty} c_n (z - z_0)^{n+\partial_2} \end{cases}, \quad \text{where} c_0 \neq 0 \tag{1.8}$$

Case II: suppose the difference of the indicial roots $(\partial_1 - \partial_2)$ yields a positive integer, the two linearly independent solutions of equation (1.4), exists in the form

$$\begin{cases} y_1(z) = \sum_{n=0}^{\infty} c_n (z - z_0)^{n+\partial_1}, \text{where } c_0 \neq 0 \\ y_2(z) = Ay_1(z)\ln(z) + \sum_{n=0}^{\infty} c_n (z - z_0)^{n+\partial_2} \end{cases} \tag{1.9}$$

Case III: suppose the difference of the indicial roots $\partial_1$and ∂_2 are equal then, the two linearly independent solutions of equation (1.4), exists and are of the form

$$\begin{cases} y_1(z) = \sum_{n=0}^{\infty} c_n (z - z_0)^{n+\partial_1}, \text{where } c_0 \neq 0 \\ y_2(z) = y_1(z)\ln z + \sum_{n=0}^{\infty} c_n (z - z_0)^{n+\partial_2} \end{cases} \tag{1.10}$$

CHAPTER TWO
NOTION OF BESSEL'S EQUATION AND THEIR PROPERTIES

In this section, we shall present the notion of Bessel's equation as a special kind of differential equation and also present their special solution as Bessel functions of different kinds and their properties.

2.1 Bessel's Differential Equation

We consider a special type of differential equation as, Gupta, (2010)

$$z^2 \frac{d^2y}{dz^2} + z\frac{dy}{dz} + (z^2 - k^2)y = 0 \qquad (2.1)$$

In equation (2.1), k can be positive or negative integer, and can also be fraction or real numbers.

The complete solution of equation (2.1) can be presented as

$$y(z) = C_1 J_k(z) + C_2 Y_k(z), \qquad (2.2)$$

where C_1 and C_2 are constants of the equation, which can be obtain, using certain boundary conditions, also $J_k(z)$ and $Y_k(z)$, respectively are Bessel's function of first and second kind.

we divide both sides of equation (2.1) by z^2, yielding

$$\frac{d^2y}{dz^2} + \frac{1}{z}\frac{dy}{dz} + \left(1 - \frac{k^2}{z^2}\right)y = 0. \qquad (2.3)$$

we compare equation (2.1.3) to equation (1.5), as

$$y''(z) + P(z)y' + Q(z)y = 0. \qquad (2.4)$$

Thus, $P(z) = \frac{1}{z}$ and $Q(z) = 1 - \frac{k^2}{z^2}$, it reveals that at some point, both $P(z)$and $Q(z)$ will be analytic, and equation (2.4) is a singular point at $z = 0$.

We now, evaluate the series solution of equation (2.1), by applying the Frobenius method, before that, we need to examine the behavior of the coefficients of equation (2.4), as

let $z P(z) = z\left(\frac{1}{z}\right) = 1$

also,

$$z^2 Q(z) = \left(1 - \frac{k^2}{z^2}\right)z^2 = z^2 - k^2 = \text{Finite value}$$

Hence, the regular singular point is at $z = 0$, we can now evaluate equation (2.1), via the Frobenius method.

2.2: Series solution of Bessel's Differential Equation

Let,

$$y(z) = \sum_{n=0}^{\infty} c_n z^{n+\partial}, \tag{2.5}$$

where n and ∂ are the indexes, note that the index ∂ is to be evaluated as the roots of the recurrence formulae of the series solution of equation (2.1).

Now, we differentiate equation (2.5), as

$$y'(z) = \frac{dy}{dz} = \frac{d}{dz}\left(\sum_{n=0}^{\infty} c_n z^{n+\partial}\right) = \sum_{n=0}^{\infty}(n+\partial)c_n z^{n+\partial-1}, \tag{2.6}$$

also, we differentiate equation (2.6), further yields

$$y''(z) = \frac{d^2y}{dz^2} = \frac{d}{dz}\left(\sum_{n=0}^{\infty}(n+\partial)c_n z^{n+\partial-1}\right)$$

$$= \sum_{n=0}^{\infty}(n+\partial)(n+\partial-1)c_n z^{n+\partial-2}. \tag{2.7}$$

Putting equations (2.5), (2.6) and (2.7) into the Bessel's equation in (2.1), we obtain

$$z^2\sum_{n=0}^{\infty}(n+\partial)(n+\partial-1)c_n z^{n+\partial-2} + z\sum_{n=0}^{\infty}(n+\partial)c_n z^{n+\partial-1}$$

$$+(z^2-k^2)\sum_{n=0}^{\infty} c_n z^{n+\partial} = 0. \tag{2.8}$$

Now, equation (2.8), becomes

$$\sum_{n=0}^{\infty}(n+\partial)(n+\partial-1)c_n z^{n+\partial} + \sum_{n=0}^{\infty} c_n z^{n+\partial} - k^2\sum_{n=0}^{\infty} c_n z^{n+\partial} +$$
$$z^2\sum_{n=0}^{\infty} c_n z^{n+\partial} = 0.$$

It means that,

$$z^{\partial}\sum_{n=0}^{\infty} c_n[(n+\partial)(n+\partial-1)+(n+\partial)-k^2]z^n + z^{\partial}\sum_{n=0}^{\infty} c_n z^{n+2} = 0$$

In the above equation, we apply change of base at the last term, by putting $n = 2 \Rightarrow n = n - 2$, then we have

$$\sum_{n=0}^{\infty} c_n[(n+\partial)(n+\partial-1)+(n+\partial)-k^2]z^n + \sum_{n=2}^{\infty} c_{n-2}z^n = 0 \tag{2.9}$$

equating the of coefficients of z^0 to zero in equation (2.9), yields

$$(\partial^2 - k^2)c_0 = 0, \quad \Rightarrow \partial = \pm k. \tag{2.10}$$

Also, equating the coefficients of first power of z to zero, in equation (2.9), we obtain

$$[(1 + \partial)^2 - k^2]c_1 = 0, \quad \Rightarrow c_1 = 0.$$

Similarly, we collect the coefficient of n^{th}-powers of z and equate to zero, we obtain

$$[(n + \partial)^2 - k^2]c_n + c_{n-2} = 0. \tag{2.11}$$

solving equation (2.2.7) , for c_n, gives

$$c_n = -\frac{1}{[(n + \partial)^2 - k^2]} . c_{n-2}, \qquad \text{for } n \geq 2. \tag{2.12}$$

Hence, equation (2.12), is called the recurrence formulae, with $c_n's$, as the coefficients, that depends on each other, since $c_1 = 0$, then the odd coefficients are equal to zero, leaving us with the only even coefficients.

2.3 Bessel Function of Different Kind

2.3.1 First kind of Bessel function For Integer Order k

From the recurrence formulae in equation (2.12), we obtain

$$c_n = -\frac{1}{[(n + \partial)^2 - k^2]} c_{n-2}, \text{ for } n \geq 2$$

Putting $\partial_1 = +k$ in the equation above, we obtain

$$c_n = -\frac{1}{n(n+2k)} c_{n-2}, \text{for } n \geq 2, \tag{2.13}$$

Now, we evaluate for n = 2, 4, 6……., equation (2.13)

For n = 2

$$c_2 = -\frac{1}{2^2.1!.(k+1)} c_0,$$

for n = 4

$$c_4 = \frac{1}{2^4.2!(k+2)(k+1)} . c_0$$

For n =6

$$c_6 = -\frac{1}{2^6.3!(k+3)(k+2)(k+1)} c_0, \ldots.,$$

set n = 2m

$$, c_{2m} = (-1)^m \frac{1}{2^{2m}.m!(k+m)\ldots, \ (k+2)(k+1)} c_0$$

Hence,

$$c_{2m} = (-1)^m \frac{1}{2^{2m}.m!(k+m)\ldots, \ (k+2)(k+1)} c_0, \tag{2.14}$$

Substituting (2.14) in the form solution in equation (2.5), yields

$$y(z) = c_0 \sum_{m=0}^{\infty} (-1)^m \frac{1}{2^{2m}.m!(k+1)(k+2)(k+3)\ldots, \quad (m+k)} . z^{2m+k} \tag{2.15}$$

For $c_0 \neq 0$, let $c_0 = \frac{1}{2^k k!}$, such that equation (2.15), becomes

$$y(z) = \sum_{m=0}^{\infty} (-1)^m \frac{1}{m!(m+k)!} \left(\frac{z}{2}\right)^{2m+k} \tag{2.16}$$

Recall, the definition of gamma as $\Gamma(p+2) = (p+1)\Gamma(p+1)$, equation (2.16) becomes

$$J_k(z) = \sum_{m=0}^{\infty} (-1)^m \frac{1}{\Gamma(m+1)\Gamma(k+m+1)} \left(\frac{z}{2}\right)^{2m+k} \tag{2.17}$$

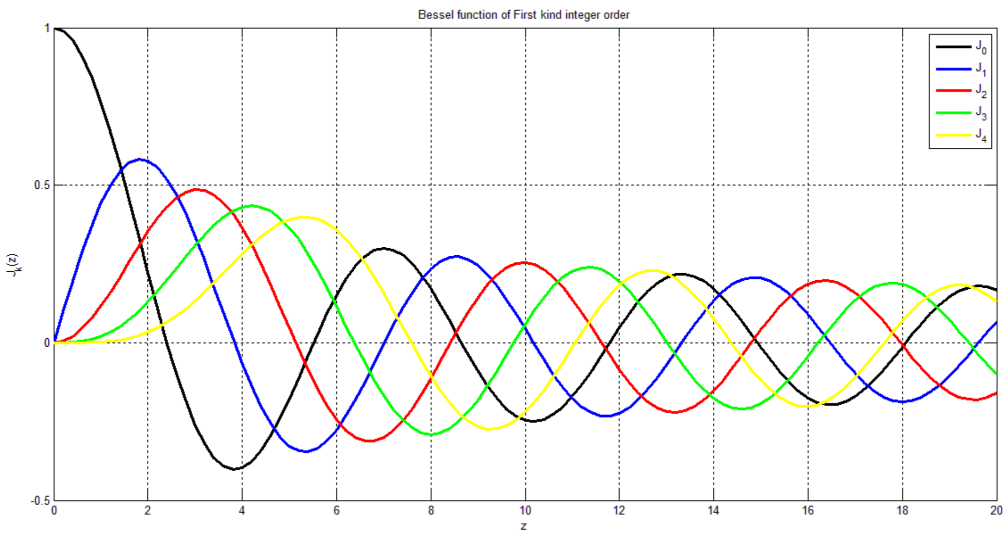

Figure 2.3.1: Integer Order, Bessel Function of First Kind.

2.3.2 Semi Integer Order k (for k = ½)

Suppose, we put $k = \pm\frac{1}{2}$, in equation (2.17), we obtain

$$J_{\pm\frac{1}{2}}(z) = \sum_{m=0}^{\infty} (-1)^m \frac{1}{m!\,\Gamma(\pm 1/2+m+1)} \left(\frac{z}{2}\right)^{2m \pm \frac{1}{2}}. \tag{2.18}$$

We can expand the summation in equation (2.18) for k = ½ and k = -½, separately, as

$$J_{1/2}(z) = \sum_{m=0}^{\infty} (-1)^m \frac{1}{m!\,\Gamma(m+3/2)} \left(\frac{z}{2}\right)^{2m+1/2}$$

$$= \sqrt{\frac{2}{\pi z}} \left(z - \frac{z^3}{3!} + \frac{z^5}{5!} -, \ldots \right)$$

$$J_{\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}} \quad \sin z, \tag{2.19}$$

for, $z > 0$.

Similarly,

$$J_{-\frac{1}{2}}(z) = \sum_{m=0}^{\infty} (-1)^m \frac{1}{m!\,\Gamma(m-1/2)} \left(\frac{z}{2}\right)^{2m-1/2}$$

$$= \sqrt{\frac{2}{\pi z}} \quad \left(1 - \frac{z^2}{2!} + \frac{z^4}{4!} -, \ldots \quad \right)$$

$$J_{-\frac{1}{2}}(z) = \sqrt{\frac{2}{\pi z}} \quad \cos z\,, \tag{2.20}$$

for, $z \geq 0$.

Hence, equation (2.19) and (2.20), are Bessel's functions, for semi integer order k.

2.3.3 Second kind of Bessel's function

For the case of $\partial_2 = -k$

Since k, in the Bessel's equation is in the form k^2, satisfying the series solution in equation (2.17), then –k must also satisfy the same series solution if the gamma functions is redefined. If –k is not an integer, then the Bessel's function $J_{-k}(z)$, is the second solution of the Bessel's differential equation of order k. Equation (2.17), becomes

$$J_{-k}(z) = \sum_{m=0}^{\infty} (-1)^m \frac{1}{\Gamma(m+1)\Gamma(-k+m+1)} \left(\frac{z}{2}\right)^{2m-k} \tag{2.21}$$

Hence, $J_{-k}(z)$ is unbounded at the origin and contains the negative powers of z and $J_k(z)$ on the hand is bounded and finite. Since –k, is not an integer, then $J_{-k}(z)$ and $J_k(z)$ are two linearly independent solutions of the Bessel's equation of order k, hence, a general solution of Bessel's differential equation, if k is a non-integer is

$$y(z) = C_1 J_k(z) + C_2 J_{-k}(z). \tag{2.22}$$

If k is an integer, then equation (2.11), differs by an integer $(\partial_1 - \partial_2 = 2k)$, the first solution is

$$y_1(z) = \sum_{m=0}^{\infty} c_{2m} z^{2m+k}, \tag{2.23}$$

also, Bessel's function of second kind, is of the form

$$y_2(z) = Y_k(z) = C_k \ln(z) \quad + \quad z^{-1} \sum_{n=0}^{\infty} D_n z^{n+k} \tag{2.24}$$

And the second solution of equation (2.23), becomes

$$y_2(z) = J_{-k}(z) = \sum_{m=0}^{\infty}(-1)^m \frac{1}{m!\Gamma(m-k)!}\left(\frac{z}{2}\right)^{2m-k}, \qquad (2.25)$$

But the expression $\Gamma(m-k+1) = \Gamma(m-k)!$, since $\Gamma(m-k+1)$ is an integer, the equation (2.25), becomes

$$y_2(z) = J_{-k}(z) = \sum_{m=0}^{\infty}(-1)^m \frac{1}{m!\Gamma(m-k+1)}\left(\frac{z}{2}\right)^{2m-k}. \qquad (2.26)$$

If $m = 0$ then $J_{-k} = 0$, since –k is not define, then it is either$+\infty$ or $-\infty$, let set m = k , so that the limit of the summation changes to

$$y_2(z) = J_{-k}(z) = \sum_{m=k}^{\infty}(-1)^m \frac{1}{m!\Gamma(m-k)!}\left(\frac{z}{2}\right)^{2m-k} \qquad (2.27)$$

Putting $(m-k) = v$, then $J_{-k}(z)$, becomes

$$y_2(z) = J_{-k}(z) = \sum_{v=0}^{\infty}(-1)^k \frac{1}{v!(l+k)!}\left(\frac{z}{2}\right)^{2v+k}$$

$$= (-1)^k J_k(z), \quad \text{for } k = 1(1)n. \qquad (2.28)$$

Now,

$y_2(z) = J_{-k}(z) = (-1)^k J_k(z)$, it shows, that k is integer, and then $J_k(z)$ and $J_{-k}(z)$ are linearly independent. Hence, equation (2.23) cannot be the general solution of the Bessel's equation.

It is easy to take the linear combination of $J_k(z)$ and $J_{-k}(z)$, by Wronskian determinant, in order to yield a second independent solution, instead of the second solution of $J_{-k}(z)$, as

$$Y_k(z) = \frac{\cos(\pi k)J_k(z) - J_{-k}(z)}{\sin(\pi k)} \qquad (2.29)$$

Equation (2.29) is called Bessel's function of second kind (Neumann function), integer order k.

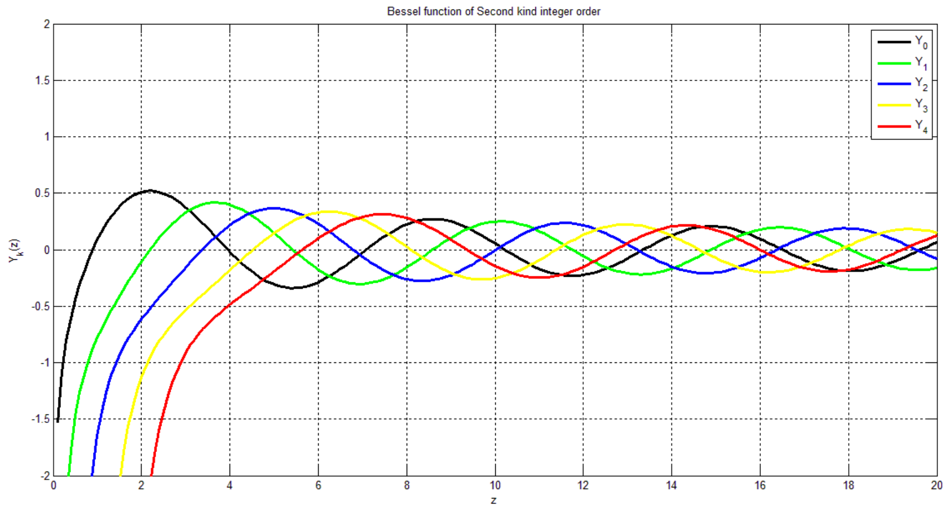

Figure 2.3.2: Integer Order Bessel Function of Second Kind.

Hence the general solution of the Bessel's differential equation in (2.1) is

$$y(z) = C_1 J_k(z) + C_2 Y_k(z) \tag{2.30}$$

If we put k = v in equation (2.29), we obtain

$$\lim_{k\to v}(Y_v(z)) = \lim_{k\to v}\left(\frac{\cos(\pi v)J_v(z) - J_{-v}(z)}{\sin(\pi v)}\right) \tag{2.31}$$

Equation (2.31), can be presented in its general form as

$$J_v(z) = J_v(z)\{\log(z) - s_N(z)\} - \sum_{m=0}^{\infty}\frac{2^{(v-m-1)}v!J_m(z)}{(v-m)m!z^{v-m}} + \sum_{m=1}^{\infty}\frac{(-1)^{(m-1)}(v+2m)}{m(v+m)}J_{v+2m}(z),$$

where,

$$s_n(z) = \left(1 + \frac{1}{2} + \frac{1}{3} +, \dots ,+\frac{1}{v}\right), \text{implying } s_0(0) = 0. \tag{2.32}$$

2.3.4 Bessel's Function of Third Kind

The Bessel function of third kind is given as the combination of the Bessel's function of first kind and second kind i.e. $J_k(z)$and $Y_k(z)$, the third kind of Bessel function is also called the Hankel function, is of the form

$$H_k^{(1)}(z) = J_k(z) + iY_k(z), \tag{2.33}$$

$$H_k^{(2)}(z) = J_k(z) - iY_k(z), \tag{2.34}$$

Where $H_k^{(1)}(z)$ and $H_k^{(2)}(z)$, stands as Hankel function of first and second kind respectively.

2.4 Bessel's modified function

Suppose the Bessel's differential equation in (2.1) can be written as

$$z^2 \frac{d^2y}{dz^2} + z\frac{dy}{dz} - (z^2 + k^2)y = 0 \qquad (2.35)$$

If we replace z to be iz, then equation (2.17), the modified Bessel's function can be written as

$$I_{\pm k}(z) = \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n \pm k)} \left(\frac{z}{2}\right)^{2n \pm k}. \qquad (2.36)$$

Equation (2.4.2), is integer order modified Bessel function of first kind.

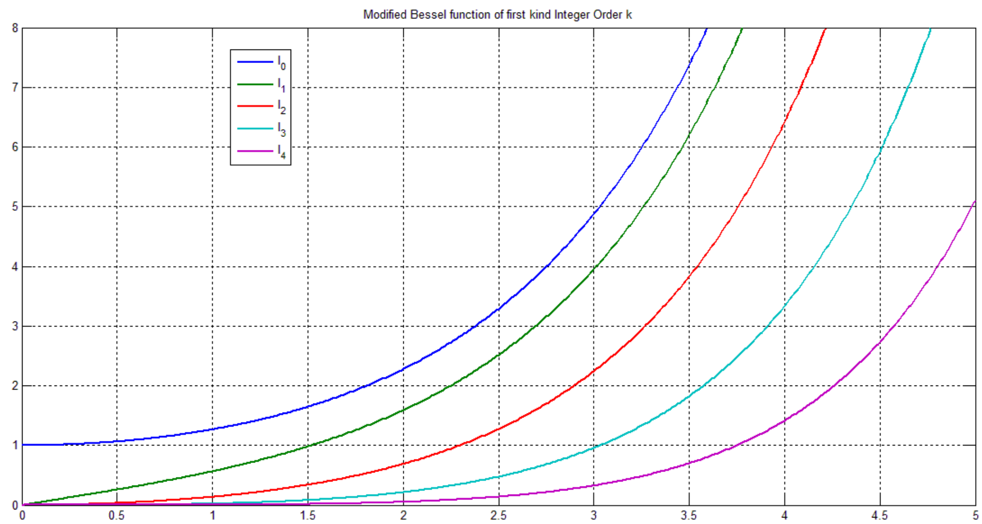

Figure 2.4.1: Integer Order First Kind, Modified Bessel Function

The general solution can be expressed as

$$Y_k(z) = C_1 I_{-k}(z) - C_2 I_k(z). \qquad (2.37)$$

C_1 and C_2, can be evaluated using the boundary conditions.

Similarly, if k is not an integer, the second linearly independent solution can be expressed as

$$K_k(z) = \frac{\pi}{2} \cdot \left(\frac{I_{-k}(z) - I_k(z)}{\sin(\pi k)}\right). \qquad (2.38)$$

Since limit as $k \rightarrow n \epsilon \mathbb{Z}$, exist.

Equation (2.38), is integer order Bessel's modified function of second kind.

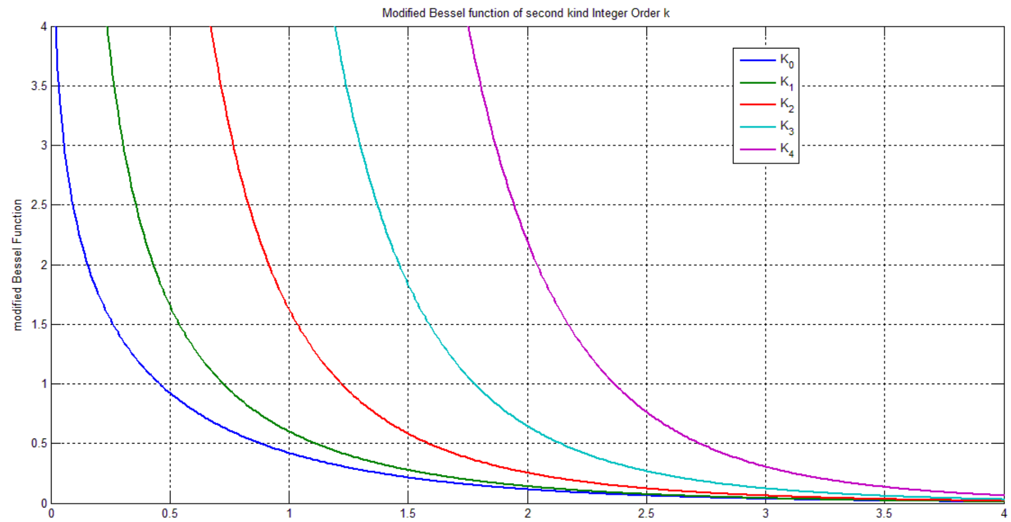

Figure 2.4.2: Integer Order Modified Bessel Function second kind.

2.5 Recurrence Relation of Bessel's Polynomial

As defined in 1.1.6, we present the basic recurrence formulae, required for further operation in Bessel's function

$$\begin{cases} zJ_k'(z) = kJ_k(z) - zJ_{k+1}(z) \\ zJ_k'(z) = -kJ_k(z) + zJ_{k-1}(z) \end{cases} \tag{2.39}$$

The recurrence formulae in (2.39), are derived as a result of differentiating equation (2.17), with respect to z.

Also,

$$\begin{cases} J_{k-1}(z) = 2J_k'(z) + zJ_{k+1}(z) \\ \frac{2k}{z}J_k(z) = J_{k-1}(z) + J_{k+1}(z) \end{cases} \tag{2.40}$$

Equations (2.40), follow directly from, equation (2.39)

Note that recurrence formulae, can be expressed in compact form as

$$\frac{d}{dz}\left[z^k J_k(z)\right] = z^k J_{k-1}(z), \tag{2.41}$$

From equation (2.17), we can show the validity of equation (2.41) as

$J_k(z) = \sum_{m=1}^{\infty} \frac{(-1)^m}{m!\Gamma(m+k+1)} \left(\frac{z}{2}\right)^{2m+k}$, substituting $J_k(z)$, in equation (2.41), yields

$$\frac{d}{dz}\left[z^k \sum_{m=1}^{\infty} \frac{(-1)^m}{m!\Gamma(m+k+1)} \left(\frac{z}{2}\right)^{2m+k}\right] = \frac{d}{dz}\left[\sum_{m=1}^{\infty} \frac{(-1)^m}{m!\Gamma(m+k+1)} \left(\frac{z}{2}\right)^{2(m+k)}\right]$$

$$\frac{dy}{dx} = \sum_{m=1}^{\infty} \frac{2(m+k)}{2} \cdot \frac{(-1)^m}{m!(m+k)\Gamma(m+k)} \left(\frac{z}{2}\right)^{2(m+k)-1} = z^k \sum_{m=1}^{\infty} \frac{(-1)^m}{m!\Gamma(m+k-1+1)} \left(\frac{z}{2}\right)^{2m+k}$$
$$= z^k J_k(z) .$$

2.6 Generating Function

We present the generating in this section, which are inter-related to the Bessel's function of integral order. $J_k(x)$ is Bessel's polynomial, which can be presented as the coefficients of powers of z^n, in the expansion of series of special function as $g(z, x)$, called the generating function in term of z^n.

Now, let

$$g(z, x) = e^{\frac{x}{2}(z-\frac{1}{z})} = \sum_{n=-\infty}^{\infty} J_n(x) z^n \qquad (2.42)$$

we shall prove equation (2.42), as follows

$$e^{\frac{x}{2}z} \times e^{-\frac{x}{2z}} = \left[\sum_{a=0}^{\infty} \left(\frac{xz}{2}\right)^a \cdot \frac{1}{a!}\right] \times \left[\sum_{b=0}^{\infty} (-1)^b \left(\frac{x}{2z}\right)^b \cdot \frac{1}{b!}\right], \qquad (2.43)$$

implying that,

$$g(z, x) = \sum_{a=0}^{\infty} \sum_{b=0}^{\infty} \frac{(-1)^b}{a!b!} \left(\frac{x}{2}\right)^{a+b} z^{a-b} \qquad (2.44)$$

Now, putting $n = r - s$, then $n = \pm\infty$ and must be independent of b

$$g(z, x) = \sum_{n=-\infty}^{\infty} \sum_{b=0}^{\infty} \left(\frac{(-1)^b}{(n+b)!b!}\right) \left(\frac{x}{2}\right)^{n+2b} z^n, \qquad (2.45)$$

Hence,

$$g(z, x) = \sum_{n=-\infty}^{\infty} \left[\sum_{b=0}^{\infty} \frac{(-1)^b}{(n+b)!b!} \left(\frac{x}{2}\right)^{n+2b}\right] z^n = \sum_{n=-\infty}^{\infty} J_n(x) z^n. \qquad (2.46)$$

2.7 Bessel's Function integral Representation: Boas,(1983).

Bessel's integral representation is of the form

$$J_n(x) = \frac{1}{\pi} \int_0^{\pi} \cos(n\theta - x \sin\theta)\, d\theta = 0, \qquad (2.47)$$

Recall, in equation (2.42),

$$g(z, x) = e^{\frac{x}{2}(z-\frac{1}{z})} = \sum_{n=-\infty}^{\infty} J_n(x) z^n,$$

Now, putting $z = e^{i\theta}$, such that the LHS, becomes

$$e^{\frac{x}{2}(z-\frac{1}{z})} = e^{\frac{x}{2}(e^{i\theta}-e^{-i\theta})} = \cos(x \sin\theta) + i \sin(x \sin\theta), \qquad (2.48)$$

from,

$$\sum_{n=-\infty}^{\infty} J_n(x)z^n = \sum_{n=-\infty}^{\infty} J_n(x)\left(e^{i\theta}\right)^n = \sum_{n=-\infty}^{\infty} J_n(x)[\cos(n\theta) + i\sin(n\theta)].$$

Expanding the above equation, yields

$$\sum_{n=-\infty}^{\infty} J_n(x)z^n = J_0(x) + 2J_2(x)\cos(2\theta) + 2J_4(x)\cos(4\theta) + \cdots,$$
$$+i[2J_1(x)\sin(\theta) + 2J_3(x)\sin(3\theta) + \cdots]. \tag{2.49}$$

Putting equation (2.49), in compact form

$$\sum_{n=-\infty}^{\infty} J_n(x)Z^n = J_0(x) + 2\sum_{k=1}^{\infty} J_{2k}(x)\cos(2k)\theta$$
$$+2i\sum_{k=1}^{\infty} J_{2k-1}(x)\sin(2k-1)\theta. \tag{2.50}$$

Equating equation (2.48) and (2.50), we obtain

$$\cos(x\sin\theta) + i\sin(x\sin\theta) = J_0(x) + 2\sum_{k=1}^{\infty} J_{2k}(x)\cos(2k)\,\theta$$
$$+2i\sum_{k=1}^{\infty} J_{2k-1}(x)\sin(2k-1)\theta. \tag{2.51}$$

Equating real and imaginary part of equations (2.51), as follows

$$\cos(x\sin\theta) = J_0(x) + 2\sum_{k=1}^{\infty} J_{2k}(x)\cos(2k)\,\theta, \tag{2.52}$$

Similarly,

$$\sin(x\sin\theta) = 2i\sum_{k=1}^{\infty} J_{2k-1}(x)\sin(2k-1)\theta, \tag{2.53}$$

Since the series in equations (2.52) and (2.53), are Fourier series of the other side of the equation, then we multiply equation (2.52) by $\cos(n\theta)$ equation (2.53) by $\sin(n\theta)$, and integrate with respect to θ, for $0 \le \theta \le \pi$.

Recall that,

$$\begin{cases} \int_0^{\pi} \cos(m\theta)\cos(n\theta)\,d\theta = \int_0^{\pi} \sin(m\theta)\sin(n\theta)\,d\theta = 0, \text{when } m \neq n \\ \int_0^{\pi} \cos^2(m\theta) = \int_0^{\pi} \sin^2(m\theta) = \frac{\pi}{2} \qquad m = n \end{cases} \tag{2.54}$$

Now, by equation (2.52),

$$\int_0^{\pi} \cos(n\theta)\cos(x\sin\theta)\,d\theta = J_0(x)\int_0^{\pi} \cos(n\theta)\,d\theta +$$
$$2\sum_{k=1}^{\infty} J_{2k}(x)\int_0^{\pi} \cos(2k)\,\theta\cos(n\theta)\,d\theta \tag{2.55}$$

When we, integrate, the first term vanishes for all values of n, and we have

$$\int_0^{\pi} \cos(n\theta)\,d\theta = 0$$

From RHS, the integral vanishes to 0, if $n \neq 2k$, so if $n = 2k$, then

$$\int_0^{\pi} \cos(n\theta)\cos(n\theta)\,d\theta = \frac{\pi}{2}; \text{ for } n = 2k : \text{even},$$

Hence,

$$\int_0^{\pi} \cos(n\theta)\,(x \sin\theta)\, d\theta = \begin{cases} \pi J_n(x)\,; & n: \text{even} \\ 0; & n: \text{odd}, \end{cases} \qquad (2.56)$$

and equation (2.53), becomes

$$\int_0^{\pi} \sin(n\theta) \sin(x \sin\theta)\, d\theta = 2i \sum_{k=1}^{\infty} J_{2k-1}(x) \int_0^{\pi} \sin(2k-1)\theta \sin\theta\, d\theta, \qquad (2.57)$$

implying that,

$$\int_0^{\pi} \sin(n\theta) \sin(x \sin\theta)\, d\theta = \begin{cases} \pi J_n(x)\,; & n: \text{odd} \\ 0; & n: \text{even}, \end{cases} \qquad (2.58)$$

adding and dividing equations (2.56) and (2.58) by π, yields

$$J_n(x) = \frac{1}{\pi} \int_0^{\pi} [\cos(n\theta - x \sin\theta) + \sin(n\theta) \sin(x \sin\theta)]\, d\theta. \qquad (2.59)$$

By using cosine formulae, we have

$$J_n(x) = \frac{1}{\pi} \int_0^{\pi} \cos(n\theta - x \sin\theta)\, d\theta = 0 \text{ , for } n = 0, 1, 2, \ldots$$

CHAPTER THREE
NOTION OF BESSEL SPHERICAL FUNCTIONS AND SCHRÖDINGER EQUATION DERIVED.

In this chapter we present the concept of Bessel's spherical function and derived the Schrödinger time independent equation. Further, describe the zero potential of a particle in spherical coordinate.

3.1 Bessel's Spherical Function

The Bessel's spherical function occurs in the radial part of the Helmholtz equation, as a result of solving the Laplace equation in the spherical coordinate.

We now, consider the Bessel's spherical equation, of the form, Boas, (1983).

$$r^2 \frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + \left(k^2r^2 - p(p+1)\right)R(r) = 0, \tag{3.1}$$

where the parameter k, originate from the Helmholtz equation and p(p+1) is a separation constant.

Now, by variable change method, equation (3.1) can be transformed as follows

we set z = kr, so that

$$r\frac{dR}{dr} = kr\frac{dR}{dz} = z\frac{dR}{dz}, \tag{3.2}$$

also,

$$r^2\frac{d^2R}{dr^2} = z^2\frac{d^2R}{dz^2}\,. \tag{3.3}$$

Putting equations (3.2) and (3.3) into equation (3.1), and rearranging we obtain

$$z^2\frac{d^2R}{dz^2} + z\frac{dR}{dz} + \left(z^2 - \left(p + \tfrac{1}{2}\right)^2\right)R(z) = 0. \tag{3.4}$$

Equation (3.4), is Bessel spherical equation of order $(p + \frac{1}{2})$, where is an integer.

Dividing equation (3.4) by z^2, yields

$$\frac{d^2R}{dz^2} + \frac{1}{z}\frac{dR}{dz} + \left(1 - \frac{\left(p+\frac{1}{2}\right)^2}{z^2}\right)R(z) = 0. \tag{3.5}$$

Equation (3.3), can be compared to the standard form of equation (1.5), as

$$y''(z) + P(z)y' + Q(z)y = 0. \tag{3.6}$$

Implying that, $P(z) = \frac{1}{z}$ and $Q(z) = 1 - \frac{(p+\frac{1}{2})^2}{z^2}$, it means that at point both $P(z)$and $Q(z)$ are analytic, and equation (3.5) is a singular point at $z = 0$.

Now, to obtain the series solution of equation (3.4), we apply the Frobenius' method, let us first analyze the behavior of the coefficients $P(z)$ and $Q(z)$, as follows

$$\text{Let, } z\,P(z) = z\left(\frac{1}{z}\right) = 1,$$

also,

$$z^2Q(z) = \left(1 - \frac{k^2}{z^2}\right)z^2 = z^2 - k^2 = \text{Finite value, where } k = p + \tfrac{1}{2}\,.$$

Hence at $z = 0$, it is a regular singular point, and we use power series method at $z = 0$, in order to obtain the solution.

3.2 Series Solution via Frobenius Method

By Frobenius method, the series solution of equation (3.4), can be obtain, which we have seen in the previous chapter.

However, if by replacing k with $(p + \frac{1}{2})$, in equation (2.17), we obtain

$$j_{p+\frac{1}{2}}(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n+p+\frac{1}{2})!}\left(\frac{z}{2}\right)^{2n+p+\frac{1}{2}}, \qquad (3.7)$$

Now, by applying Legendre duplication formulae in equation (3.7), that is

$$n!\left(n + \tfrac{1}{2}\right)! = 2^{-2n-1}\sqrt{\pi}\,(2n+1)!, \qquad (3.8)$$

we obtain,

$$j_p(z) = \sqrt{\frac{\pi}{2z}}\sum_{n=0}^{\infty} \frac{(-1)^{2n+2p+1}(n+p)!}{\sqrt{\pi}(2n+2p+1)!n!}\left(\frac{z}{2}\right)^{2n+p+\frac{1}{2}} = 2^p z^p \sum_{n=0}^{\infty} \frac{(-1)^{2n+2p+1}(n+p)!}{\sqrt{\pi}(2n+2p+1)!n!}(z)^{2n}. \qquad (3.9)$$

Implying that,

$N_{p+\frac{1}{2}}(z) = (-1)^{p+1}J_{-p-\frac{1}{2}}(z)$, and by equation (2.17), we have

$$J_{-p-\frac{1}{2}}(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n-p-\frac{1}{2})!n!}\left(\frac{z}{2}\right)^{2n-p-\frac{1}{2}}. \qquad (3.10)$$

From equation (2.29), we can deduce that, $\cos\left(p + \frac{1}{2}\right)\pi = 0$, then equation (3.10), becomes

$$N_p(z) = (-1)^{p+1}\frac{2^p\sqrt{\pi}}{z^{p+1}}\sum_{n=0}^{\infty} \frac{(-1)^n}{\left(n-p-\frac{1}{2}\right)!n!}\left(\frac{z}{2}\right)^{2n-p-\frac{1}{2}}. \qquad (3.11)$$

By equations (3.10) and (3.11), we obtain

$$j_p(z) = \sqrt{\frac{\pi}{2t}} J_{p+\frac{1}{2}}(z), \tag{3.12}$$

$$n_p(z) = \sqrt{\frac{\pi}{2t}} N_{p+\frac{1}{2}}(z). \tag{3.13}$$

Hence, the general solution of equation (3.1), can be presented as

$$y(z) = C_1 j_p(z) + C_2 n_p(z). \tag{3.14}$$

where $j_p(z)$ and $n_p(z)$, are spherical Bessel function and Neumann spherical Bessel function or (regular and irregular functions) respectively, the constant C_1 and C_2 are evaluated, by applying the boundary conditions.

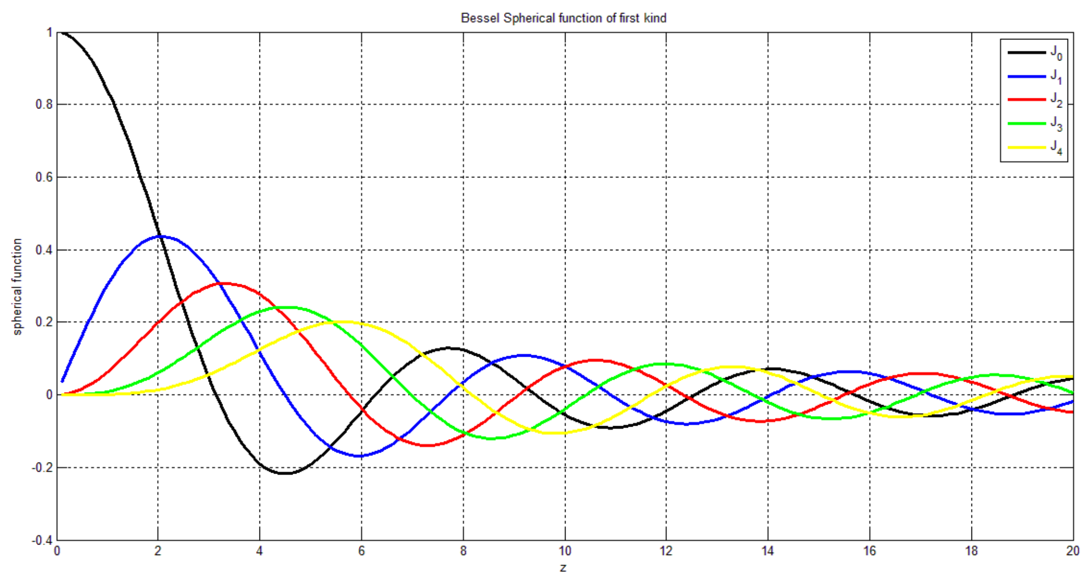

Figure 3.2.1: Spherical Bessel function of First kind

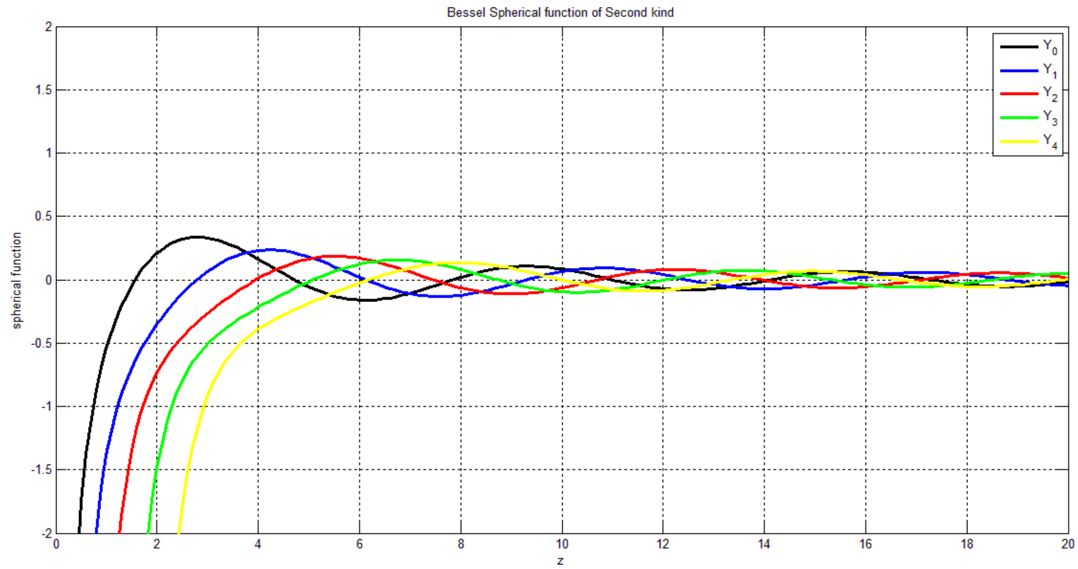

Figure 3.2.2: Spherical Bessel function of Second Kind

Similarly, we can express the spherical Hankel Bessel functions of first and second kind as follows

$$h_p^{(1)}(z) = \sqrt{\frac{\pi}{2z}} H_{p+\frac{1}{2}}^{(1)}(z) \; = j_p(z) + in_p(z), \tag{3.15}$$

Also,

$$h_p^{(2)}(z) = \sqrt{\frac{\pi}{2z}} H_{p+\frac{1}{2}}^{(2)}(z) \quad = j_p(z) - in_p(z). \tag{3.16}$$

3.3 Derivation of Schrödinger Time Independent Equation: Griffrth, (1995).

We consider a particle moving in the x-coordinate with a velocity and mass m, momentum P_x, and energy E, by assuming that the wave particle is represented by a complex variable $\psi(x,t)$ we first derive the one-dimensional time dependent Schrödinger equation, with the speed of the particle smaller to the speed of light. The total energy is the kinetic energy $\left(\frac{P_x}{2m}\right)$ and the potential energy $V(x)$.

Implying that,

$$E = \frac{P_x}{2m} + V(x), \tag{3.17}$$

Since the wave function is $\psi(x,t)$, multiplying equation (3.17) by the wave function, we obtain

$$E\psi(x,t) = \frac{P_x}{2m}\psi(x,t) + V(x)\psi(x,t), \tag{3.18}$$

where,

$$\psi(x,t) = Ae^{\frac{i}{\hbar}(xP_x - Et)}. \tag{3.19}$$

We differentiate equation (3.19), partially twice with respect to x, yields the following

$$\frac{\partial\psi(x,t)}{\partial x} = \left(\frac{i}{\hbar}\right)P_x Ae^{\frac{i}{\hbar}(xP_x - Et)} = \left(\frac{i}{\hbar}\right)P_x\psi(x,t), \tag{3.20}$$

also,

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = \left(\frac{i}{\hbar}\right)P_x\frac{\partial\psi(x,t)}{\partial x}, \quad \text{but } \frac{\partial\psi(x,t)}{\partial x} = \left(\frac{i}{\hbar}\right)P_x\psi(x,t),$$

implying, $\frac{\partial^2\psi(x,t)}{\partial x^2} = \left(\frac{i}{\hbar}\right)P_x.\left(\frac{i}{\hbar}\right)P_x.\psi(x,t) = \frac{-1}{\hbar^2}P_x^2\psi(x,t)$

We obtain

$$P_x^2\psi(x,t) = -\hbar^2\frac{\partial^2\psi(x,t)}{\partial x^2}, \tag{3.21}$$

similarly, we can differentiate equation (3.19), partially, with respect to t, then we obtain

$$\frac{\partial\psi(x,t)}{\partial t} = \left(\frac{i}{\hbar}\right)(-E)Ae^{\frac{i}{\hbar}(xP_x - Et)} = -\left(\frac{i}{\hbar}\right)E\psi(x,t).$$

Transposing the above equation, we obtain

$$-\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t} = E\psi(x,t). \tag{3.22}$$

Putting equations (3.23) and (3.22), into equation (3.18), yields

$$-\frac{\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = -\left(\frac{\hbar}{i}\right)\frac{\partial\psi(x,t)}{\partial t}. \tag{3.23}$$

Hence, equation (3.23) is the time-dependent Schrödinger equation.

Equation (3.23), can be separated into the time dependent part and time independent part, keeping E as a constant and the V(x) is treated as a function of x only.

Let,

$$\psi(x,t) = U(x)G(t), \tag{3.24}$$

Where U(x) and G(t), are the time dependent and time independent functions, respectively.

We differentiate equation (3.24) partially with respect to x twice as

$$\frac{\partial\psi(x,t)}{\partial x} = \frac{dU(x)}{dx}G(t), \quad \textit{a}\text{lso}, \quad \frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{d^2U(x)}{dx^2}G(t). \tag{3.25}$$

Similarly, we differentiate with respect to t as

$$\frac{\partial\psi(x,t)}{\partial t} = \frac{dG(t)}{dt}U(x). \tag{3.26}$$

Putting equations (3.24), (3.25) and (3.26) into equation (3.23), we obtain,

$$-\frac{\hbar}{2m}.\frac{d^2U(x)}{dx^2}G(t) + V(x)U(x)G(t) = -\frac{\hbar}{i}\frac{dG(t)}{dt}U(x).$$

We multiply both sides by $\frac{1}{U(x)G(t)}$, yields

$$-\frac{\hbar}{2mU(x)}\frac{d^2U(x)}{dx^2} + V(x) = -\frac{\hbar}{iG(t)}\frac{dG(t)}{dt} \tag{3.27}$$

Clearly, equation (3.27) is separated into the function with partial variable x and the time function respectively.

Substituting equation (3.25), into equation (3.22) yields

$E\psi(x,t) = -\frac{\hbar}{i}U(x)\frac{dG(t)}{dt}$, but $\psi(x,t) = U(x)G(t)$,

implying that,

$EU(x)G(t) = -\frac{\hbar}{i}U(x)\frac{dG(t)}{dt}$, we multiply through by $\frac{1}{U(x)G(t)}$, giving

$$E = -\frac{\hbar}{iG(t)}\frac{dG(t)}{dt}. \tag{3.28}$$

inserting equation (3.28) into equation (3.27), we obtain

$$-\frac{\hbar}{2mU(x)}\frac{d^2U(x)}{dx^2} + V(x) = E,$$

multiplying by $\frac{2U(x)m}{\hbar}$, we have

$$\frac{d^2U(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]U(x) = 0. \tag{3.29}$$

Hence, equation (3.29), is the Schrödinger time independent equation.

3.4 Particle of Zero (0) Potential Described

We now, consider a Schrödinger equation of a zero potential i.e. V(x) =0, of the form

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + E\right]\psi_E(r) = 0 \tag{3.30}$$

with,

$$V(r) = \begin{cases} 0, 0 \leq r \leq a \\ \infty, \quad r > a \end{cases} \tag{3.31}$$

Suppose the solution of equation (3.30), is a wave function of the form

$$\psi\left(k, \ell, \frac{m}{r}\right) = V_{k,\ell}(r)Y_{\ell,m}(\theta, \phi) \tag{3.32}$$

Then we have

$$\left[-\frac{\hbar^2}{2mr}\partial_r^2 + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + E_{\ell,m}\right]V_{k,\ell}(r) = 0, \quad (3.33)$$

it means, that $E = \frac{\hbar^2k^2}{2mr} \geq 0$, we substitute $E = \frac{\hbar^2k^2}{2mr}$, in equation(3.33) and then multiply through by $-\frac{2mr}{\hbar^2}$, then we obtain

$$\left[\partial_r^2 - \frac{\ell(\ell+1)}{r^2} + k^2\right]V_{k,\ell}(r) = 0, \quad (3.34)$$

we substitute$V_{k,\ell}(r) = j_\ell(kr)$, to be the solution of equation (3.34), then we now let a new variable $x = kr$, we obtain

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + 1\right]xj_\ell(x) = 0. \quad (3.35)$$

Substituting equation (3.31), into equation (3.35), two solutions exists for small r, (I.e. as $r \to 0$), which are regular and irregular solution respectively

$$j_\ell(x) = x^\ell, \text{and } n_\ell(x) = x^{-\ell-1}, \quad (3.36)$$

similarly, the general solution as $r \to \infty$, is

$$j_\ell(x) = \frac{1}{x}\ (\sin(x+\beta)), \quad (3.37)$$

for some β, putting $f_\ell(x) = j_\ell(x), n_\ell(x)$, in equation (3.35), we obtain

$$\left[\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} - \frac{\ell(\ell+1)}{x^2}\right]f_\ell(x) = 0. \quad (3.38)$$

Hence, $\sin(x+\beta)$ can be express as a solution of equation (3.35), in the form of an infinite power series as

$$j_\ell(x) = t^\ell y(x^2), \text{implying that, } y(x^2) = \sum_{n=0}^{\infty} c_n x^{2n}, \quad (3.39)$$

The coefficient of the expansion, can be evaluated by putting equation (3.39) into equation (3.35), where y in equation (3.39) is depending upon x^2 , which follows from

$$\frac{d}{dt}[x^{\ell+1}y(x)] = \frac{dy(x)}{dx}.x^{\ell+1} + (\ell+1)y(x).$$

Also,

$$\frac{d}{dx}\left[\frac{dy(x)}{dx}.x^{\ell+1} + (\ell+1)y(x)\right] = \frac{d^2y(x)}{dx^2}.x^{\ell+1} + (\ell+1)x^\ell.\frac{dy(x)}{dx} + \ell(\ell+1)x^{\ell-1}y(x) +$$
$$(\ell+1)x^\ell.\frac{dy(x)}{dx} = \frac{d^2y(x)}{dx^2} + (\ell+1)\frac{2}{x}\frac{dy(x)}{dx} + \ell(\ell+1)x^{\ell-1}y(x).$$

Comparing the above equation with equation (3.35), we have

$$\left[\frac{d^2}{dx^2} + (\ell + 1)\frac{2}{x}\frac{d}{dx} + 1\right] y(x) = 0, \tag{3.40}$$

we introduce an independent variable as $u = x^2$, then

$$\frac{1}{x}\frac{d}{dx} = 2\frac{d}{du}\text{, also } \frac{d^2}{dx^2} = 4u\frac{d^2}{du^2} + 2\frac{d}{du.}$$

Putting the above into equation (3.40), and evaluating we obtain

$$\left[\frac{d^2}{du^2} + \frac{2\ell+3}{2u}\frac{d}{du} + \frac{1}{4u}\right] y(u) = 0. \tag{3.41}$$

Putting $y(x^2) = \sum_{n=0}^{\infty} c_n x^{2n}$, into equation (3.41) and $u = x^2$, we have

$$\sum_{n=0}^{\infty}\left[c_n n(n-1)u^{n-2} + \tfrac{1}{2}(2\ell + 3)c_n u^{n-1} + \tfrac{1}{4}c_n u^{n-1}\right] = 0,$$

Changing the base of the first term, will yield

$$\sum_{n=0}^{\infty}\left[c_{n+1} n(n-1) + \tfrac{1}{2}(2\ell + 3)c_{n+1} + \tfrac{1}{4}c_n\right]u^{n-1} = 0.$$

If $u^{n-1} \neq 0$, we obtain the recurrence formulae of the form:

$$c_{n+1} = -\frac{1}{2}.\frac{c_n}{(n+1)(2n+2\ell+3)} \tag{3.42}$$

For $n = 0,1,2..$ and $\ell = 0,1,2,..$, respectively.

For $n = 0$, For $n = 1$, For $n = 2$,

$$c_1 = -\frac{1}{2}.\frac{c_0}{1!(2\ell+3)}, \qquad c_2 = \frac{1}{4}.\frac{c_0}{2!(2\ell+3)(2\ell+5)}, \qquad c_3 = -\frac{1}{6}.\frac{c_0}{3!(2\ell+3)(2\ell+5)(2\ell+7)}.$$

We choose

$$c_0 = \frac{x^\ell}{1.3.5...,(2\ell+1)} \tag{3.43}$$

Then,

$$j_\ell(x) = \frac{x^\ell}{1.3.5...,(2\ell+1)}\left[1 - \frac{x^2/2}{1!(2\ell+3)} + \frac{(x^2/2)^2}{2!(2\ell+3)(2\ell+5)} - + \cdots\right], \tag{3.44}$$

Similarly,

$$n_\ell(x) = \frac{1.3.5...,(2\ell+1)}{x^{\ell+1}}\left[1 - \frac{x^2/2}{1!(2\ell+3)} + \frac{(x^2/2)^2}{2!(2\ell+3)(2\ell+5)} - + \cdots\right]. \tag{3.45}$$

Hence, equations (3.44) and (3.45) are regular and irregular spherical Bessel functions respectively.

We can express equations (3.44) and (3.45) further in factorial form as an infinite sum as;

Recall the definition of factorial in chapter one as

$$\frac{1}{2}.\frac{3}{2}.\frac{5}{2},\dots,\left(\ell+\frac{1}{2}\right)\text{, implying that } \Gamma\left(\ell+\frac{1}{2}\right)=\sqrt{\pi}.\frac{1}{2}.\frac{3}{2}.\frac{5}{2},\dots,\left(\ell+\frac{1}{2}\right)$$

we can express equation (3.45) as

$$j_\ell(x)=\frac{1}{\frac{1}{2}\cdot\frac{3}{2}\cdots\left(\ell+\frac{1}{2}\right)}\left[1+\frac{(ix/2)^2}{1!(2\ell+\frac{3}{2})}+\frac{(ix/2)^4}{2!(2\ell+\frac{3}{2})(2\ell+\frac{5}{2})}+\cdots\right],$$

from the above we can deduce that

$$j_\ell(x)=\frac{\sqrt{\pi}}{2}\left(\frac{t}{2}\right)^\ell\sum_{n=0}^{\infty}\frac{(ix/2)^{2n}}{n!\Gamma(n+1+\ell+\frac{1}{2})}. \quad (3.46)$$

Similarly, we can write equation (3.45) as

$$n_\ell(x)=\frac{2\ell}{\sqrt{\pi t^{\ell+1}}}\Gamma\left(\ell+\frac{1}{2}\right)\left[1+\frac{(ix/2)^2}{1!\left(\frac{1}{2}-\ell\right)}+\frac{(ix/2)^4}{2!\left(\frac{1}{2}-\ell\right)\left(\frac{3}{2}-\ell\right)}+\cdots\right]. \quad (3.47)$$

But $t=\ell+\frac{1}{2}$, and since $\Gamma(\ell)\Gamma(1-\ell)=\frac{\pi}{\sin\pi t}$, implying that $\Gamma\left(\ell+\frac{1}{2}\right)=(-1)^\ell\frac{\pi}{\Gamma(\ell+\frac{1}{2})}$, and we can write equation (3.47) as

$$n_\ell(x)=(-1)^{\ell+1}\sqrt{\pi}\frac{2^\ell}{z^{\ell+1}}\left[\frac{I}{\Gamma\left(\frac{1}{2}-\ell\right)}+\frac{(ix/2)^2}{1!\Gamma\left(\frac{1}{2}-\ell\right)\left(\frac{1}{2}-\ell\right)}+\frac{(ix/2)^4}{2!\Gamma\left(\frac{1}{2}-\ell\right)\left(\frac{1}{2}-\ell\right)\left(\frac{3}{2}-\ell\right)}+,\dots\right],$$

Hence,

$$n_\ell(x)=(-1)^{\ell+1}\frac{\sqrt{\pi}}{2}\left(\frac{2}{z}\right)^{\ell+1}\sum_{n=0}^{\infty}\frac{(ix/2)^{2n}}{n!\Gamma(n+1-\ell-\frac{1}{2})}. \quad (3.48)$$

3.5 Relationship of Spherical Bessel's Functions

Before discussing the relationship in spherical Bessel function we take a look the reason why we have two independent solutions of equation (3.35), via the Wronskian method which follows from equations (3.44) and (3.45), as

$$W\left(j_\ell(x),n_\ell(x)\right)=j_\ell(x)\frac{d}{dx}n_\ell(x)-\frac{d}{dx}j_\ell(x)n_\ell(x). \quad (3.49)$$

Let y_1 and y_2, be the solution of equation (3.35), then we have

$$\frac{d^2}{dx^2}y_{1,2}=-\frac{t}{2}\frac{d}{dx}y_{1,2}+\frac{\ell(\ell+1)}{x^2}y_{1,2}+y_{1,2}.$$

By the identity of the above equation we can write

$$\frac{d}{dx}W(y_1,y_2)=-\frac{2}{x}W(y_1,y_2)=\frac{d}{dx}\ln(W)=\frac{d}{dx}\ln\left(\frac{1}{x^2}\right)=\ln(W)=\frac{A}{x^2}$$

Where A is constant for cases of $y_1 = j_\ell(x)$ and $y_2 = n_\ell(x)$, which is evaluated via the expansion of equations (3.44) and (3.45) and putting $A = 1$, we obtain

$$W\left(j_\ell(x), n_\ell(x)\right) = \frac{1}{x^2}. \tag{3.50}$$

Since the Wronskian of the regular and irregular solution is not equal to zero, it means that the two solution of equation (3.35) are linearly independent.

In equation (3.38) the function $f_\ell(x)$ can be written in its simplest form as

$f_\ell(x) = F_{\ell+1}(x)$, implying that

$$\frac{d}{dx}(f_\ell(x)) = \frac{1}{\sqrt{x}}\frac{d}{dx}F_{\ell+\frac{1}{2}}(x) - \frac{1}{2t\sqrt{x}}F_{\ell+\frac{1}{2}}(x) ,$$

we obtain

$$\frac{d^2}{dx^2}(f_\ell(x)) = \frac{1}{\sqrt{x}}\frac{d^2}{dx^2}F_{\ell+\frac{1}{2}}(x) - \frac{1}{t\sqrt{t}}\frac{d}{dx}F_{\ell+\frac{1}{2}}(x) + \frac{3}{4t^2\sqrt{x}}F_{\ell+\frac{1}{2}}(x). \tag{3.51}$$

Evaluating equation (3.51), lead to

$$\left[\frac{d^2}{dx^2} + \frac{1}{t}\frac{d}{dx} - \frac{k^2}{x^2} + 1\right]F_k(x) = 0, \tag{3.52}$$

Where $k = \ell + \frac{1}{2}$, hence the solution equation (3.52) can be written as

$$J_k(x) = \left(\frac{x}{2}\right)^k \sum_{n=0}^{\infty} \frac{(ix/2)^{2n}}{n!\Gamma(n+k+1)}. \tag{3.53}$$

Equation (3.53), is a regular Bessel function, which is obtain via the power series expansion similar to that of equation (3.44). From the above equation it is easy to deduce that $J_k(x)$ and $J_{-k}(x)$ are linearly independent since $k = \ell + \frac{1}{2}$.

Now,

$$W\left(J_{\ell+\frac{1}{2}}(x), J_{-\ell-\frac{1}{2}}(x)\right) = (-1)^\ell \frac{2}{\pi x}, \tag{3.54}$$

relating $J_{\ell+\frac{1}{2}}(x)$ and $J_{-\ell-\frac{1}{2}}(x)$ to the solution in equations (3.46 and (3.47), we obtain

$$j_\ell(x) = \sqrt{\frac{\pi}{2t}}J_{\ell+\frac{1}{2}}(x), \tag{3.55}$$

$$n_\ell(x) = (-1)^{\ell+1}\sqrt{\frac{\pi}{2t}}J_{-\ell-\frac{1}{2}}(x). \tag{3.56}$$

From equation (3.55) and (3.56), we can obtain the Hankel spherical Bessel function of first and second kind, which is also a solution of equation (3.35), and are of the form

$$h_\ell^{(1,2)}(x) = \sqrt{\frac{\pi}{2t}} H_{\ell+\frac{1}{2}}^{(1,2)}(x), \tag{3.57}$$

from equations (3.38) and (3.56), we can obtain the Bessel regular function as

$$j_\ell(x) = {}^1\!/_2 \left(h_\ell^1(x) + h_\ell^2(x)\right). \tag{3.58}$$

we can also deduce that, that equation (3.56) also a relationship with the irregular spherical Bessel function as

$$n_\ell(x) = (-1)^{\ell+1} \sqrt{\frac{\pi}{2t}} \left(H^1_{-\left(\ell+\frac{1}{2}\right)}(x) + H^1_{-\left(\ell+\frac{1}{2}\right)}(x) \right). \tag{3.59}$$

Since $H^{(1,2)}_{-(\ell+\frac{1}{2})}(x) = \pm i(-1)^\ell H^{(1,2)}_{\ell+\frac{1}{2}}(x)$, and by equation (3.58), the above equation becomes

$$h_\ell^1(x) = j_\ell(x) + i n_\ell(x), \tag{3.60}$$

similarly,

$$H_\ell^1(x) = j_\ell(x) + i n_\ell(x). \tag{3.61}$$

CHAPTER FOUR
APPLICATION OF BESSEL FUNCTIONS

In this section, we now dissect the Laplace wave equation, in their respective coordinates of cylindrical and spherical systems and compare them to Schrödinger time independent equation, in order to relate their general solutions.

4.1 Application In Cylindrical Well.

We now consider, a particle moving in two dimensions with mass m and potentials of zero inside the box and infinite potential outside the box, the Laplace equation in (1.2) represent this problem in the cylindrical coordinates. Relating equation (1.2) with the Schrödinger time independent equation, we have

$$-\frac{\hbar^2}{2m}\left[r\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2}\right]=E\psi(r,\varphi). \tag{4.1}$$

Assume the solution of equation (4.1) is

$$\psi(r,\varphi)=R(r)T(\varphi). \tag{4.2}$$

we differentiate equation (4.2), partially by each dependent variable and then fix the result in equation (4.1) as

$$-\frac{\hbar^2}{2m}\left[T(\varphi)\ \frac{1}{R(r)}\frac{\partial}{\partial r}\left(r\frac{dR(r)}{dr}\right)+\frac{1}{r^2}R(r)\frac{d^2T(\varphi)}{d\varphi^2}\right]=ER(r)T(\varphi.)$$

we multiply the above equation by $\frac{1}{R(r)T(\varphi)}$ and $-\frac{2m}{\hbar^2}$ and rearranging we obtain

$$\frac{1}{rR(r)}\frac{\partial}{\partial r}\left(r\frac{dR(r)}{dr}\right)+\frac{1}{T(\varphi)r^2}\frac{d^2T(\varphi)}{d\varphi^2}=-\frac{2mE}{\hbar^2}. \tag{4.3}$$

Putting $k^2=\frac{2mE}{\hbar^2}$ and we multiply equation (4.3) by r^2, we obtain

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right)+k^2r^2+\frac{1}{T(\varphi)}\frac{d^2T(\varphi)}{d\varphi^2}=0. \tag{4.4}$$

we can split equation (4.4), into their respective depend variables of r and φ, and introduce the constant of separation as $\pm\mu^2$, we obtain

$$\frac{1}{T(\varphi)}\frac{d^2T(\varphi)}{d\varphi^2}=-\mu^2, \tag{4.5}$$

similarly,

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right)+k^2r^2=\mu^2\ .$$

We multiply by R(r) and rearrange, and get

$$\frac{d^2R}{dr^2}r^2 + r\frac{dR}{dr} + (k^2r^2 - \mu^2)R(r) = 0. \quad (4.6)$$

Equation (4.5), is also known as the harmonic oscillator. Solving and normalizing the solution gives

$$T(\varphi) = \sqrt{\frac{1}{2\pi}}e^{i\mu\varphi}\,, \quad (4.7)$$

Equation (4.6), is also known as the radial part of equation (4.1), and is the same type of equation with equation (2.1), whose are those of Bessel functions of different kinds.

The general solution is

$$R(r) = C_1 J_\mu(kr) + C_2 N_\mu(kr). \quad (4.8)$$

C_1 and C_2 in equation (4.1.8) are constanst, which are evaluated via application of boundary conditions $J_\mu(kr)$ and $N_\mu(kr)$ are integer order, first kind and Neumann Bessel function respectively in cylindrical coordinates.

We now apply the given conditions of the problem, to equation (4.8), that is when the potential inside the box is i.e. $r = 0$, then $J_\mu(kr)$, is finite and when the potential outside the box is infinite i.e. $r = \infty$, then $N_\mu(kr)$, is infinite at the origin, which shows that $C_2 = 0$, and we have equation (4.8), reduces to

$$R(r) = C_1 J_\mu(kr). \quad (4.9)$$

Also, if the radius inside the box $R(r) = 0$, then $J_\mu(kr) = 0$, which implies that kr, is the zeros of Bessel functions. We can put $kr_1 = \beta_{\mu,n}$, which enables us to calculate their respective zeros, μ, is the order of the Bessel function and n is the corresponding zero. From this we can evaluate the individual energy of the system by putting k in place of $\beta_{\mu,n}$, that is $k = \frac{2mE}{\hbar^2}$, and then evaluating further to have

$$E_{\mu,n} = \frac{\beta_{\mu,n}^2\hbar^2}{2mr_1^2}. \quad (4.10)$$

Thus, the general solution of equation (4.4), is

$$\psi_\mu(r,\varphi) = C_1 J_\mu\left(\frac{\beta_{\mu,n}r}{r_1}\right)\sqrt{\frac{1}{2\pi}}e^{i\mu\varphi}. \quad (4.11)$$

Evaluating equation (4.11), in a closed form is difficult, however, by a way of example to show the important of zeros of Bessel function, in the role of the above equation, assume that order of the function $\mu = 2$ and the correspond zero $n = 1$ to be $r_1 = 5.13562$ (from table of Bessel function), which serves as the radius of the box, we re-write equation (4.11) as an individual solution in the form

$$\psi_2(r,\varphi) = C_{\mu,n} J_2\left(\frac{\beta_{2,1} r}{r_1}\right)\sqrt{\frac{1}{2\pi}} e^{i\mu\varphi}. \tag{4.12}$$

The constant $D_{\mu,n}$, can be evaluated via normalization and applying the boundary condition in order to obtain their numerical solution by the help of a mathematical software.

4.2 Application in Spherical Well

If we relate equation (1.3) along with the problem

$$V(r) = \begin{cases} 0, & \text{if } r < a \\ \infty, & \text{if } r > a, \end{cases} \tag{4.13}$$

Equation (1.3), can be express as Schrödinger time independent equation as

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\left(\frac{\partial^2\psi}{\partial\varphi^2}\right)\right] + V(r)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi). \tag{4.14}$$

We assume the solution of equation (4.14) to be

$$\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi). \tag{4.15}$$

We differentiate equation (4.15), with respect to their respective dependent variables of r, θ, and φ, and putting the result of differentiation along with equation (4.15), in equation (4.14), we obtain

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2(\theta)}\left(\frac{\partial^2 Y}{\partial\varphi^2}\right)\right]$$
$$+V(r)R(r)Y(\theta,\varphi) = ER(r)Y(\theta,\varphi).$$

We multiply the above equation by, $\frac{1}{R(r)Y(\theta,\varphi)}$ and $-\frac{2mr^2}{\hbar^2}$ and rearranging we obtain

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E)R + \frac{1}{Y}\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial Y}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\left(\frac{\partial^2 Y}{\partial\varphi^2}\right)\right] = 0.$$

The above equation can be split into functions in order of their dependent variable, and then introduce $\ell(\ell+1)$ as the constant of separation, we obtain

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E)R = \ell(\ell+1). \tag{4.16}$$

Similarly,

$$\frac{1}{Y}\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial Y}{\partial\theta}\right)+\frac{1}{r^2\sin^2(\theta)}\left(\frac{\partial^2 Y}{\partial\varphi^2}\right)\right]=-\ell(\ell+1). \qquad (4.17)$$

Again we can split equation (4.17), into two separate functions according to their dependent variable of θ and φ , by assuming the solution of (4.17) as

$$Y(\theta,\varphi)=\Theta(\theta)\phi(\varphi). \qquad (4.18)$$

We differentiate equation (4.18), with respect to their respective dependent variable of θ, and φ, and putting the result of differentiation along with equation (4.18), in equation (4.17), we obtain two separate functions as

$$\frac{d^2\phi}{d\varphi^2}+\mu^2\phi=0, \qquad (4.19)$$

also,

$$\sin(\theta)\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{d\Theta}{\partial\theta}\right)+\ell(\ell+1)\sin^2(\theta)\Theta=\mu^2\Theta. \qquad (4.20)$$

Solving equation (4.19), we get

$$\phi(\varphi)=\sqrt{\frac{1}{2\pi}}\,e^{i\mu\varphi}, \qquad (4.21)$$

where $A=\sqrt{\frac{1}{2\pi}}$, is evaluated via normalization method.

Similarly, we have the solution of equation (4.20), as the Legendre function as

$\Theta_\ell^\mu \propto P_\ell^\mu(\cos(\theta))$, where the range $-\ell,\dots,\ell$ is restricted by μ, and we obtain

$$P_\ell^\mu(x)=(1-x)^{\frac{abs(\mu)}{2}}\left(\frac{d}{dx}\right)^{abs(\mu)}, \qquad (4.22)$$

where $P_\ell^\mu(x)$, is the Legendre function in equation (4.22).

We combine the functions in equations (4.21) and (4.22), to the spherical harmonic function as

$$Y_\ell^\mu(\theta,\varphi)=\left(\frac{(2\ell+1)(\ell-abs(\mu))}{4\pi(\ell+abs(\mu))}\right)^{\frac{1}{2}}e^{i\mu\varphi}P_\ell^\mu(\cos(\theta)). \qquad (4.23)$$

Now, inserting $U(r)=rR(r)$, in equation (4.16), we obtain

$$-\frac{\hbar^2}{2m}\frac{d^2U}{dr^2}+\left(V(r)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)U(r)=EU(r), \qquad (4.24)$$

Equation (4.24), is the radial equation similar to one dimensional Schrödinger time independent equation, with effective potential as

$$V_{eff}=V(r)+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}, \qquad (4.25)$$

Substituting $r=0$, in equation (4.24), $\psi(r,\theta)=0$, but if $r<a$, we obtain

$$\frac{d^2\mathrm{U}}{\mathrm{dr}^2} = \left(\frac{\ell(\ell+1)}{\mathrm{r}^2} - \mathrm{k}^2\right)\mathrm{U(r)} = \mathrm{EU(r)}, \tag{4.26}$$

By putting $\mathrm{k} = \sqrt{\frac{2\mathrm{mE}}{\hbar}}$, then we present the general solution of equation (4.26), as

$$\mathrm{U(r)} = C_1 \mathrm{j}_\ell(\mathrm{kr}) + C_2 \mathrm{n}_\ell(\mathrm{kr}). \tag{4.27}$$

$$\text{where} \begin{cases} \mathrm{j}_\ell(\mathrm{kr}) = (-\mathrm{z})^\ell \left(\frac{1}{\mathrm{z}}\frac{\mathrm{d}}{\mathrm{dz}}\right)^\ell \frac{\sin(\mathrm{z})}{\mathrm{z}}, \\ \mathrm{n}_\ell(\mathrm{kr}) = -(-\mathrm{z})^\ell \left(\frac{1}{\mathrm{z}}\frac{\mathrm{d}}{\mathrm{dz}}\right)^\ell \frac{\cos(\mathrm{z})}{\mathrm{z}}. \end{cases} \tag{4.28}$$

For small values of r in equation (4.27), the Bessel spherical function ($\mathrm{j}_\ell(\mathrm{kr})$) is finite at the origin and Neumann spherical function ($\mathrm{n}_\ell(\mathrm{kr})$), is infinite at the origin, it means $C_2 = 0$, the equation (4.27) reduces to

$$\mathrm{U(r)} = C_1 \mathrm{j}_\ell(\mathrm{kr}). \tag{4.29}$$

Since, $\mathrm{U(a)} = 0$, then $\mathrm{j}_\ell(\mathrm{kr}) = 0$, which also implies the zeros of a Bessel function. By putting $\mathrm{kr}_1 = \beta_{\ell,\mathrm{n}}$, where $\beta_{\ell,\mathrm{n}}$ is the n^{th}, zero of spherical Bessel function of the ℓ^{th}order, means for each order ℓ, we have the corresponding zero of the function as n.

Now, we can put $\mathrm{k} = \frac{\beta_{\ell,\mathrm{n}}}{\mathrm{r}_1}$ and recall that $\mathrm{k} = \frac{\sqrt{2\mathrm{mE}}}{\hbar}$, by this assertion, the individuals zeros and energies of the function can be evaluated from the relation

$$\mathrm{E}_{\ell,\mathrm{n}} = \frac{\beta_{\ell,\mathrm{n}}^2 \hbar^2}{2\mathrm{mr}_1^2}. \tag{4.30}$$

Hence, the general solution of the function is

$$\psi_{\ell,n,\mu}(\mathrm{r},\theta,\varphi) = C_{\ell,\mathrm{n}} \mathrm{J}_\ell\left(\frac{\beta_{\ell,\mathrm{n}}\mathrm{r}}{\mathrm{r}_1}\right) \mathrm{Y}_\ell^\mu(\theta,\varphi), \tag{4.31}$$

where $\mathrm{C}_{\ell,\mathrm{n}}$, is a constant, which can be evaluated by normalization of the function, by using particular examples of the zeros of the spherical Bessel function.

CHAPTER FIVE
NUMERICAL RESULTS

In this section, we shall present the numerical solutions, for a mixed problem of a Schrödinger equation. This is necessary when the analytic solution becomes too problematic to obtain. Numerical solution means, in simple terms to present the approximate solution of a problem.

Numerical solution plays very important role in the world of applied mathematics and engineering. We shall use the modified Gauss elimination method, to present the approximate solution for the mixed problem of Schrödinger equation, via the use of Matlab programming language to realize our computations. The approximate solution of the first and second order accuracy difference scheme shall be presented.

5.1. Mixed Problem For a Schrödinger Equation

We now consider the mixed problem for the Schrödinger equation

$$\begin{cases} iu_t(t,x) + x^2 u_{xx}(t,x) + xu_x(t,x) + (x^2 - \frac{1}{4})u(t,x) + u(t,x) = 0, \\ 0 \le t \le \pi, 0 \le x \le \pi, \\ u(0,x) = \sqrt{\frac{2}{\pi x}}\sin(x), 0 \le x \le \pi, \\ u(t,0) = u(t,\pi) = 0, 0 \le t \le \pi. \end{cases} \quad (5.1)$$

Solving problem (5.1) partially, by separation of variables, we obtain the analytic solution for the problem as

$$u(t,x) = e^{it}\sqrt{\frac{2}{\pi x}}\sin(x). \quad (5.2)$$

For numerical solution of (5.1), we consider the first order accuracy difference scheme

$$\begin{cases} i\frac{u_n^k - u_n^{k-1}}{\tau} + x_n^2 \frac{2u_{n+1}^k - 2u_n^k + u_{n-1}^k}{h^2} + x_n \frac{u_{n+1}^k - u_{n-1}^k}{2h} + (x_n^2 + \frac{3}{4})u_n^k = 0, \\ 0 \le k \le N, x_n = nh, 1 \le n \le m-1, mh = \pi, N\tau = \pi, \\ u_n^0 = \sqrt{\frac{2}{\pi x}}\sin(x), x_n = nh, 1 \le n \le m, \\ u_0^k = u_m^k = 0, 0 \le k \le N. \end{cases} \quad (5.3)$$

we can express the above system in (5.3) in it matrix form as

$$\begin{cases} A_n u_{n+1} + B_n u_n + C_n u_{n-1} = D\gamma_n, 1 \le n \le m-1 \\ u_0^k = u_m^k = 0. \end{cases} \tag{5.4}$$

here,

$$A_n = \begin{bmatrix} 0 & 0 & 0 & . & . & 0 & 0 & 0 \\ 0 & a & 0 & . & . & 0 & 0 & 0 \\ 0 & 0 & a & . & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & . & a & 0 \\ 0 & 0 & 0 & . & . & . & 0 & a \end{bmatrix}_{(N+1)\times(N+1)}$$

$$B_n = \begin{bmatrix} 1 & 0 & 0 & . & . & 0 & 0 & 0 \\ c & d & 0 & . & . & 0 & 0 & 0 \\ 0 & c & d & . & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & 0 & c & d \\ 0 & 0 & 0 & . & . & 0 & 0 & c \end{bmatrix}_{(N+1)\times(N+1)}$$

$$C_n = \begin{bmatrix} 0 & 0 & 0 & . & . & 0 & 0 & 0 \\ 0 & b & 0 & . & . & 0 & 0 & 0 \\ 0 & 0 & b & . & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & 0 & b & 0 \\ 0 & 0 & 0 & . & . & 0 & 0 & b \end{bmatrix}_{(N+1)\times(N+1)}$$

where $a = \frac{x_n^2}{h^2} + \frac{x_n}{2h}; c = \frac{i}{\tau}; d = \frac{i}{\tau} - \frac{2x_n^2}{h^2} + x_n^2 + \frac{3}{4}; b = \frac{x_n^2}{h^2} - \frac{x_n}{2h}$

$$\gamma_n = \begin{bmatrix} \gamma_n^0 \\ \gamma_n^1 \\ \vdots \\ \gamma_n^N \end{bmatrix}_{(N+1)\times 1}, \left\{ \begin{array}{l} \gamma_n^k = 0, 1 \le k \le N, \\ \gamma_n^0 = \sqrt{\dfrac{2}{\pi x}} \sin(x), x = x_n, \end{array} \right\},$$

The identity matrix $D = I_{N+1}$,

$$u_s = \begin{bmatrix} u_s^0 \\ u_s^1 \\ \vdots \\ u_s^N \end{bmatrix}_{(N+1)\times 1}, s = n-1, n, n+1.$$

The system in (5.4), will be evaluated to obtain the approximate solution, via the modified Gauss elimination method. The solution of the matrix can be presented as

$$u_n = \alpha_{n+1} u_{n+1} + \beta_{n+1}, n = m-1, \ldots, 2, 1, u_n = 0.$$

Where $u_n = u_m = 0$, $\alpha, (j = 1, \ldots, m-1)$, are square matrices of $(N+1) \times (N+1)$ and $\beta, (j = 1, \ldots, m-1)$, is $(N+1) \times 1$ column matrix and

$$Q = (B_n + C_n \alpha_{n+1})^{-1}$$
$$\alpha_n = Q A_n$$
$$\beta_n = Q(D_n \gamma_n - C_n \beta_{n+1}) \tag{5.5}$$

The error of the system can be computed by

$$E_m^N = \max_{1\le k\le N-1} \left(\sum_{n=1}^{M-1} \left| u(t_k, x_n) - u_n^k \right|^2 h \right)^{\frac{1}{2}} \tag{5.6}$$

implying that $u(t_k, x_n)$ is the exact solution of the problem and u_n^k is the numerical solution of the problem at $u(t_k, x_n)$ and the numerical result is as follows

Table 5.1: Error result for first order of accuracy difference scheme.

Difference schemes	m=N=20	m=N=40	m=N=80
First order numerical result	0.1831	0.0893	0.0419

From the numerical result presented in Table5.1, when we doubled the value of N and m, the error obtained is decrease by a factor of approximately ½, for the first order accuracy difference scheme.

Similarly, for the numerical solution of the mixed problem in (5.1), we consider the second of order accuracy difference scheme

$$\begin{cases} i\dfrac{u_n^k - u_n^{k-1}}{\tau} + \dfrac{1}{2}(x_n^2 \dfrac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{h^2} + x_n \dfrac{u_{n+1}^k - u_{n-1}^k}{2h} + (x_n^2 + \dfrac{3}{4})u_n^k \\ +x_n^2 \dfrac{u_{n+1}^{k-1} - 2u_n^{k-1} + u_{n-1}^{k-1}}{h^2} + \dfrac{u_{n+1}^{k-1} - u_{n-1}^{k-1}}{2h} + (x_n^2 + \dfrac{3}{4})u_n^{k-1}) = 0, \\ 0 \le k \le N, x_n = nh, 1 \le n \le m-1, mh = \pi, N\tau = \pi, \\ u_n^0 = \sqrt{\dfrac{2}{\pi x}} \sin(x), x_n = nh, 1 \le n \le m, \\ u_0^k = u_m^k = 0, 0 \le k \le N. \end{cases} \quad (5.7)$$

Equation (5.7) can be represented in its matrix form of (5.4)

where,

$$A_n = \begin{bmatrix} 0 & 0 & 0 & . & . & 0 & 0 & 0 \\ e_1 & e_2 & 0 & . & . & 0 & 0 & 0 \\ 0 & e_1 & e_2 & . & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & e_1 & e_2 & 0 \\ 0 & 0 & 0 & . & . & 0 & e_1 & e_2 \end{bmatrix}_{(N+1)\times(N+1)}$$

$$B_n = \begin{bmatrix} 1 & 0 & 0 & . & . & 0 & 0 & 0 \\ f_1 & f_2 & 0 & . & . & 0 & 0 & 0 \\ 0 & f_1 & f_2 & . & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & f_1 & f_2 & 0 \\ 0 & 0 & 0 & . & . & 0 & f_1 & f_2 \end{bmatrix}_{(N+1)\times(N+1)}$$

$$
C_n = \begin{bmatrix}
0 & 0 & 0 & . & . & 0 & 0 & 0 \\
g_1 & g_2 & 0 & . & . & 0 & 0 & 0 \\
0 & g_1 & g_2 & . & . & 0 & 0 & 0 \\
. & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . \\
0 & 0 & 0 & . & . & g_1 & g_2 & 0 \\
0 & 0 & 0 & . & . & 0 & g_1 & g_2
\end{bmatrix}_{(N+1)\times(N+1)}
$$

where $e = e_1 = e_2 = \frac{x_n^2}{2h^2} + \frac{x_n}{4h}; f = f_1 = f_2 = -\frac{i}{\tau} - \frac{x_n^2}{h^2} + \frac{x_n^2}{2} + \frac{3}{8};$

$g = g_1 = g_2 = \frac{x_n^2}{2h^2} - \frac{x_n}{4h}$

Applying (5.5), we can obtain the approximate solution, via the modified Gauss elimination method.

The error of the system can be computed, using (5.6), the solution is as follows

Table 5.2: Error result for second order of accuracy difference scheme.

Difference schemes	m=6,N=108	m=12,N=300	m=24,N=1200
Second order numerical result	0.0646	0.0144	0.0037

From the numerical result above, when we doubled the value of m and increased the value of N, the error obtained is decrease by a factor of approximately ¼, for the second order accuracy difference scheme.

5.2 Conclusion

In this thesis, we examined a study of Bessel functions and applications to the solution of Schrödinger time independent equation in cylindrical and spherical well. We dissects the Laplace Equation in their respective coordinates and then relate them with Schrödinger time independent equation and presents their solutions and also discussed the nature of their zero potentials inside and infinite potential outside the box.

We presented the behavior of their solutions as they relates to Schrödinger time independent equation, along these regions. This revealed that the individual zeros and energies of the function can be evaluated due to the interrelation of their solutions inside and outside the box.

Furthermore, we presented the numerical solution, for mixed problem of a Schrödinger equation, for but first and second order accuracy scheme, in which the error analysis is decreased by an estimated factor in each case.

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APPENDICES

APPENDIX 1: MATLAB IMPLEMENTATION CODE FOR FIRST ORDER ACCURACY DIFFERENCE SCHEME

```
%first order
N=80;
M=80;
tau=pi/N;
h=pi/M;
A=zeros(N+1,N+1,M+1);
C=zeros(N+1,N+1,M+1);
B=zeros(N+1,N+1,M+1);

for n=1:M+1;

for i=2:N+1;
   x=(n-1)*h ;
   A(i,i,n)=((x^2)/(h^2))+(x/(2*h));
end;
A;
end
for n=1:M+1;

for i=2:N+1;
   x=(n-1)*h ;
      C(i,i,n)=((x^2)/(h^2))-(x/(2*h));
end;
C;
end
for n=1:M+1;
```

```
for j=2:N+1 ;
    x=(n-1)*h ;
 B(j,j-1,n)=(complex(0,-1))/(tau);
B(j,j,n)=((complex(0,1))/(tau))-(2*(x^2)/(h^2))+(x^2)+(3/4);
end;
B(1,1,n)=1;
B;
end
D=eye(N+1,N+1);
fii=zeros(N+1,N+1);

for n=2:M+1
    x=(n-1)*h;
for k=2:N;
    fii(k,n) =0;
fii(1,n) =((2/(pi*x))^(1/2))*sin(x);
end;
end
fii(1,1) =0;
alpha{1}=zeros(N+1,N+1);
betha{1}=zeros(N+1,1);

for j=2:M;
Q=inv(B(:,:,j)+C(:,:,j)*alpha{j-1});
alpha{j}=-Q*A(:,:,j);
betha{j}=Q*(D*(fii(:,j))-C(:,:,j)*betha{j-1});
end;
U=zeros(N+1,M+1);
for j=M:-1:1
   U(:,j)=alpha{j}*U(:,j+1)+betha{j};
```

```
end

'EXACT SOLUTION OF THIS PROBLEM';
for j=2:M+1 ;
for k=1:N+1 ;
es(k,j) =exp((complex(0,1))*(k-1)*tau)*((2/(pi*(j-1)*h))^(1/2))*sin((j-1)*h);
end;
end;
%figure ;
%m(1,1)=min(min(U))-0.01;
%m(2,2)=nan;
%surf(m);
%hold;
%surf(es) ; rotate3d ;axis tight;
%title('EXACT SOLUTION');
%figure ;
%surf(m);
%hold;
%surf(U) ; rotate3d ;axis tight;
%title('FIRST ORDER');
% .ERROR ANALYSIS.;
maxes=max(max(abs(es))) ;
maxerror=max(max(abs(es-U)));
relativeerror=maxerror/maxes;
cevap1 = [maxerror,relativeerror]
```

APPENDIX 2: MATLAB IMPLEMENTATION CODE FOR SECOND ORDER ACCURACY DIFFERENCE SCHEME

```
%Second order
N=80;
M=80;
tau=pi/N;
h=pi/M;
A=zeros(N+1,N+1,M+1);
C=zeros(N+1,N+1,M+1);
B=zeros(N+1,N+1,M+1);

for n=1:M+1;

for i=2:N+1;
    x=(n-1)*h ;
    A(i,i-1,n)=(1/2)*(((x^2)/(h^2))+(x/(2*h)));
    A(i,i,n)=(1/2)*(((x^2)/(h^2))+(x/(2*h)));
end;
A;
end
for n=1:M+1;

for i=2:N+1;
 x=(n-1)*h ;
 C(i,i,n)=(1/2)*(((x^2)/(h^2))-(x/(2*h)));
 C(i,i-1,n)=(1/2)*(((x^2)/(h^2))-(x/(2*h)));
end;
C;
end
for n=1:M+1;
```

```
for j=2:N+1 ;
    x=(n-1)*h ;
B(j,j,n)=((complex(0,1))/(tau))-(1/2)*((2*(x^2)/(h^2))-(x^2)-(3/4));
B(j,j-1,n)=-((complex(0,1))/(tau))-(1/2)*((2*(x^2)/(h^2))-(x^2)-(3/4));
end;
B(1,1,n)=1;
B;
end
D=eye(N+1,N+1);
fii=zeros(N+1,N+1);
for n=2:M+1
    x=(n-1)*h;
for k=2:N;
    fii(k,n) =0;
fii(1,n) =((2/(pi*x))^(1/2))*sin(x);
end;
end
fii(1,1) =0;
alpha{1}=zeros(N+1,N+1);
betha{1}=zeros(N+1,1);

for j=2:M;
Q=inv(B(:,:,j)+C(:,:,j)*alpha{j-1});
alpha{j}=-Q*A(:,:,j);
betha{j}=Q*(D*(fii(:,j))-C(:,:,j)*betha{j-1});
end;
U=zeros(N+1,M+1);
for j=M:-1:1
   U(:,j)=alpha{j}*U(:,j+1)+betha{j};
end
```

```
'EXACT SOLUTION OF THIS PROBLEM';
for j=2:M+1 ;
for k=1:N+1 ;
es(k,j) =exp((complex(0,1))*(k-1)*tau)*((2/(pi*(j-1)*h))^(1/2))*sin((j-1)*h);
es(k,1)=0;
end;
end;
%figure ;
%m(1,1)=min(min(U))-0.01;
%m(2,2)=nan;
%surf(m);
%hold;
%surf(es) ; rotate3d ;axis tight;
%title('EXACT SOLUTION');
%figure ;
%surf(m);
%hold;
%surf(U) ; rotate3d ;axis tight;
%title('FIRST ORDER');
% .ERROR ANALYSIS.;
maxes=max(max(abs(es))) ;
maxerror=max(max(abs(es-U)));
relativeerror=maxerror/maxes;
cevap1 = [maxerror,relativeerror]
```