UNIVERSITI TEKNOLOGI MARA

TECHNICAL REPORT

A STUDY OF SCHRÖDINGER EQUATION
- ANALYTICAL AND NUMEROV METHOD

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IN THE NAME OF ALLAH, THE MOST GRACIOUS,THE MOST MERCIFUL

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ABSTRACT

Schrödinger equation is one of the basic equations of quantum mechanics. In this project, the series solution is used to solve the time independent Schrödinger equation for harmonic oscillator potential. The power-series expansion is used to calculate the energy of harmonic oscillators. The Numerov method is used to solve the Schrödinger in infinite spherical well. The results of harmonic oscillator and infinite spherical well are obtained by using MATLAB. The graphs of the wave function and probability distribution of a harmonic oscillator for n=0, 1,2,3,4,5,10 are plotted. The wave function of harmonic oscillator potential has greater peaks near both edges and have a smallest amplitude and loop length near x = 0. The graphs of the radial part of wave function of infinite spherical well are plotted for angular quantum number (ℓ) =0, 1, 2, 3. The power series is suitable to calculate the wave function of harmonic oscillator potential and the Numerov method can be used to solve the radial equation for some values of ℓ.

1. INTRODUCTION

Many problems in areas of application, such as theoretical physics, chemical physics, physical chemistry, astrophysics, electronics and others is reduce to a system of order ODEs of Schrödinger equation,(Avdelas &Simos,2001). Schrödinger's equation is fundamental equation of nonrelatives quantum mechanisms. It involves ordinary differential equations of second order in which the first derivative does not appear explicitly. Its important for physics is obvious to solve them both efficiently and reliably by numerical methods (Simos, 1997). The time-independent Schrödinger equation is one of the basic equations of quantum mechanics.

In recent years there has been a lot of activities in the area of numerical solution of the radial or one-dimensional solution. David (2006), defined the Schrödinger equation time independent as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi(x)=E\,\psi(x) \qquad (1)$$

where $\hbar$ is Planck's constant, m is the mass of the particle, ψ is the (complex valued) wave function that we want to find, $V(x)$ is a function describing the potential energy at each point x, and E is the energy, a real number, sometimes called eigenenergy.
David (2006), also defined that the time independent Schrodinger equation has the form correlates to

$$H\psi=E\,\psi(x) \qquad (2)$$

where the eigenvalues of H are possible energies E of the system and the eigenfunctions of H are wave functions.

In most cases one would use numerical methods or some rough approximations to solve (1) (Binesh et al., 2010). However, for a few limited forms of simple potentials energy function of the one–dimensional Schrödinger equation can be solved analytically. According to Alastair (2008), there are various forms of Schrödinger potentials can be studied such as the infinite square well, the finite square well and harmonic oscillator potential. Besides that, there are other complicated potential exist in Schrödinger equation for example Anharmonic Oscillator Potential and Symmetric double well Potential (Fack & Berghe, 1987). Other than that, Hydrogen atom, and spherical Coordinates of Schrödinger equation also can be studied (Robert ,2006).

The harmonic oscillator is a familiar problem classical mechanics. The harmonic oscillator form is the basis to a many problems, for example the solution to vibrational motion in molecules and in infra-red spectroscopy. Beside that, the harmonic oscillator also plays an important role in the quantum theory of solids (Alaistair, 2008).