UNIVERSITI PUTRA MALAYSIA

MATHEMATICA PACKAGES FOR SOLVING SCHRODINGER EQUATION WITH ONE DIMENSIONAL RECTANGULAR POTENTIALS

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By

ABUBAKER AHMED MOHAMED SIDDIG

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Master of Science

January 2003

Dedicated to

My

Parents

Brothers

and Sisters.

Abstract of the thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirements for the degree of Master of Science.

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Faculty: Science and Environmental Studies

The determination of eigenvalues and their related eigenfunctions is one of the central problems of quantum mechanics. In this work, the problem of finding energy eigenvalues and eigenfunctions are aptly demonstrated with one dimensional systems of infinite double square well potential, finite double square well potential, rectangular potential hole between two walls and asymmetric square well potential. We develop Mathematica packages for which the Schrodinger equations are solved for each model. The solutions are obtained by graphical and numerical methods in these packages. The packages are easy to use; the user does not need to know the details of the packages in order to use them but the user has a direct control over parameters of the models. Eigenvalues and eigenfunctions have been obtained for various well depths and widths as well as various barrier widths. They are shown to have appropriate limiting solutions. The packages are stable, fast, efficient and can serve as useful tools for teaching systems of one dimensional rectangular potential, in quantum mechanics.

Abstrak tesis yang dikemukan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Master Sains

PAKEJ MATHEMATICA UNTUK MENYELESAIKAN PERSAMAAN SCHRODINGER DENGAN KEUPAYAAN SEGI EMPAT SATU DIMENSI

Oleh

ABUBAKER AHMED MOHAMED SIDDIG

January 2003

Pengerusi: **Profesor Madya Hishamuddin Zainuddin, Ph.D.**

Fakulti: **Fakulti Sians dan Pengajian Alam Sekitar**

Penentuan nilai eigen dan fungsi eigen berpadanan merupakan salah satu masalah utama mekanik kuantum. Dalam penyelidikan ini, masalah mencari nilai eigen dan fungsi eigen tenaga sedemikian ditunjukkan melalui sistem-sistem satu dimensi dengan keupayaan dwiperigi segi empat tak terhingga, keupayaan dwiperigi segi empat terhingga, keupayaan lubang segi empat di antara dua dinding dan keupayaan perigi segi empat asimetri. Kami telah bangunkan pakej-pakej Mathematica yang menyelesaikan persamaan Schroedinger bagi setiap model. Penyelesaian telah diperolehi melalui kaedah grafik dan numerik dalam pakej tersebut. Pakej-pakej ini mudah digunakan; pengguna tidak perlu pengetahuan terperinci untuk menggunakan pakej ini tetapi mempunyai kawalan terus ke atas parameter model. Nilai dan fungsi eigen telah diperolehi untuk pelbagai lebar dan dalam perigi, dan juga untuk pelbagai lebar sawar. Ditunjukkan fungsi-fungsi ini mempunyai bentuk penyelesaian yang sesuai dalam had tertentu. Pakej-pakej yang telah dibangunkan adalah stabil, cepat, efisien dan mampu berperanan sebagai alat

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bantu pengajaran system keupayaan segi empat satu dimensi dalam mekanik kuantum.

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LIST OF SYMBOLS and ABBREVIATIONS

Symbol

κ	Wave number
k	Wave number
β	Wave number
α	Wave number
ψ	Wave function
$\hbar$	Planck's constant
$\hat{H}$	Hamiltonian operator
E	Eigenvalue
O	Operator
V	Potential dept

CHAPTER I

INTRODUCTION

Understanding Quantum Mechanics

Quantum mechanics is the theoretical framework of motion and interaction of particles at the small scales where the discrete nature of the physical world becomes important. Every quantum particle is characterized by a wave function. Erwin Schrodinger developed the differential equation which describes the evolution of those wave functions. By using Schrodinger equation, scientists can find the wave function which solves a particular problem in quantum mechanics. Unfortunately, it is usually impossible to find an exact closed solution to the equation; exact solutions are known only for special cases of potential energy V(x), and one discussed in standard quantum mechanics books (Baym, 1969, Bohm, 1979, Eisberg, 1961, Griffiths, 1995 and Merzbacher, 1998). So certain techniques are used in order to obtain an answer for the particular problem. Approximations techniques are very useful for treating systems of certain potentials for which the Schrodinger equation cannot be solved in a closed form. Variational methods and perturbations theory are two examples of the most powerful techniques. Hartree-Fock theory provides another good technique for the molecular system. The numerical approaches are widely used with the aid of large computing machines. In recent years, computers offer interactive capabilities and rapid graphical results. Nowadays modern computers give the possibility to visualize the solutions of Schrodinger equation.

Computation

Computation is a form of communication that transcends applications and technological boundaries, and is a tool that could promote discovery, scientific understanding and learning. Historically, computational quantum mechanics other than numerical ones have not been emphasized. However with the development of personal computers, several programs for quantum mechanics now exist. In recent years there have appeared softwares can serve as engine of high-level language for technical computing such as Matlab and Mathematica. With the development of Mathematica software (Wolfram, 1999), students will more find more opportunities to learn quantum mechanics interactively. In this work, the choice of Mathematica is made because of its flexibility and elegance in handling the three computational modes namely numerical, symbolic and graphical.

Wave mechanics

There are several possible formalisms of quantum mechanics, commonly referred as Heisenberg matrix mechanics and Schrodinger wave mechanics. Schrodinger developed his theory of wave mechanics by writing down an equation known as the Schrodinger equation. It was subsequently shown that Heisenberg and Schrodinger approaches were equivalent, although Schrodinger turned out to be easier to visualize with for most applications. In his formalism, the central idea is de Broglie's wave-particle duality hypothesis.

One-Dimensional potentials

In quantum mechanics, the measurement of a physical quantity E can result only in one of the eigenvalues of the corresponding operator $\hat{o}$. The eigenvalues of $\hat{o}$ forming the spectrum of the operator may be discrete, continuous or both. The eigenfunctions of $\hat{o}$ form a complete basis which may be used to expand an arbitrary wave function. The expansion coefficients can be used to determine the probability of finding the system in an eigenstate of the operator $\hat{o}$ with eigenvalue E. One of the fundamental quantities of a quantum dynamical system is its energy. The Schrodinger equation is an example of an eigenvalue equation where the operator corresponding to energy is the Hamiltonian operator of the system. Solving this second order differential Schrodinger equation is the main task essentially giving the wave functions of the particles (Rae, 1992).

The Infinite Double Potential Square Well

The potential function we are investigating is true to its name; it possesses two wells on either end of a barrier. As a consequence of this shape, the particle will feel free of any force in the well, except for when it reaches any sharp drop or rise in the potential function, where it feels an instantaneous infinite force. Classically speaking, this force simply leads to elastic collisions similar to those of gas particles reflecting of the walls of a solid container. But quantum mechanics predicts a different phenomena. A particle bound initially deep within one well will slowly leak out and find itself sometimes in one well, and sometimes the other. We are considering the cases that do not slosh or evolve in time.

The Finite Double Square Well

The study of the double square well potential has become more popular in seventies. A similar problem has been considered using double harmonic oscillator potential and the solutions to the time independent Schrodinger equation are the parabolic cylindrical functions. The problem was considered using the WKB method and approximate solution is obtained. Further, in an article by Lapidus (Lapidus 1971), an analytic treatment of the double potential well problem is discussed where twin δ functions are used for the potential. This model is of two identical finite square wells and separated by a distance a. The double square well potential crudely represents the electronic part of the potential energy of a diatomic molecule. The square wells replace the near-coulomb potentials experienced by an electron in the vicinity of either of two identical charged nuclei. Of course, real molecules generally have several electrons, which are not restricted to one-dimensional motion. However, most of the wave functions for diatomic molecules can be illustrated by this model, which has the advantage that it can be solved exactly.

The Rectangular Hole between two Walls

The rectangular potential hole is a square potential well between deep walls. In this model there are two possibilities for energy eigenvalues, the bound states $E<0$ and the positive energy eigenvalues $E>0$ (Flugge, 1971). There are discrete

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eigenvalues for a finite distance between the hole and the walls l, which with increasing l form an increasingly dense level system.

Asymmetrical Square Well

In the asymmetrical finite square well the potential function appear as lop sided and here the eigenvalue problem appears in a different manner depending on the value of E compared to the potentials V_1 and V_2. We shall consider the spectrum of the energy values $E<V_2$, for which it discrete. A particle's wavefunction in this potential well can be characterised by the depth of the well, potential value of region one and region three, energy of the particle and the mass of the particle.

Significance of the Work

The development of Mathematica packages of one dimensional potential models can assist students' understanding of selected topics in quantum mechanics incorporating computation several ways. First, it can trigger the students' interest through interactively solving Schrodinger equation. Secondly, by representing the eigenvalues and eigenfunctions graphically and numerically the students will hopefully develop a feeling for the behavior of these quantum mechanical systems that cannot be gained by conventional means. Even though Mathematica has played an essential role in this work, the student or user is not required to have any knowledge of Mathematica apart from initializing the package which is simple.

Objective

The principal purpose of this research is to develop Mathematica packages which calculate the energy eigenvalues and eigenfunctions numerically and graphically for systems with the following potential wells

- Infinite double potential square well.
- Finite double square well.
- The rectangular hole between two walls
- Asymmetrical square well.