NUMERICAL SOLUTION OF NONLINEAR SCHRÖDINGER EQUATION USING CRANK-NICOLSON METHOD

MD NOMAN UDDIN

A dissertation submitted in partial fulfilment of the
requirements for the award of the degree of
Master of Science

Faculty of Science
Universiti Teknologi Malaysia

FEBRUARY 2020

DEDICATION

To my parents and my friends

ACKNOWLEDGEMENT

First and foremost, I would like to thank all lecturers of UTM for their assistance since the beginning of my Masters education. I am also immensely grateful to my supervisor, Dr. Shazirawati Mohd Puzi, for meeting me on a regular basis and sharing her valuable comments. I'm also thankful to my co-supervisor, Dr. Hang See Pheng, for her constructive criticism of my dissertation. In addition, I want to give a special thanks to Dr. Yeak Su Hoe for helping me with the programming part of my dissertation.

I would like to thank my fellow Masters' students for their cooperation and their friendship. Furthermore, I would like to express my gratitude to the staff of UTM library.

Finally, I must express my profound indebtedness to my parents for giving me their unwavering support and continuous encouragement throughout the years of my education at UTM. This accomplishment would not have been possible without them. Thank you.

ABSTRACT

The nonlinear Schrödinger equations (NLS) are used in modeling several physical phenomena such as Bose-Einstein condensation, laser beam transmissions, deep water turbulence, and solitary wave propagation in optical fibers. Solving NLS equation resulting in a wave function that makes it easier to examine the behavior and performance of physical systems or chemical reactions. There are several methods that can be used to solve the nonlinear Schrödinger equation. In this study, one dimensional nonlinear Schrödinger equation was solved by Crank-Nicolson method with Dirichlet boundary condition and symmetric cyclic tridiagonal matrix using MATLAB. The Crank-Nicolson scheme is used as it is one of the adaptable, fast, and robust techniques for integrating the time-dependent Schrödinger equation. In addition, the operational framework for finite difference scheme and stability analysis for this technique are presented. Lastly, the performance of the Crank-Nicolson scheme is analyzed by computing the error between the estimated and the exact solution. It is shown that both results from numerical scheme and exact solution have good agreement.

ABSTRAK

Persamaan Schrödinger talc linear (NLS) digunakan dalam pemodelan fenomena fizikal seperti pemeluwapan Bose-Einstein, transmisi pancaran laser, pergolakan air dalam, penyebaran gelombang tunggal dalamda gentian optik. Penyelesaian kepada persamaan NLS membolehkan kajian terhadap kelakuan dan prestasi sistem fizikal atau tindak balas kimia dapat dilakukan dengan lebih mudah. Terdapat banyak kaedah yang boleh digunakan untuk menyelesaikan persamaan Schrödinger talc linear. Dalam kajian ini, teknik Crank-Nicolson dengan nilai sempadan Dirichlet dan matrik tiga pepenjuru dengan kitaran simetri digunakan untuk menyelesaikan persamaan Schrödinger tidak linear satu dimensi dangan MATLAB. Skim Crank-Nicolson digunakan kerana ia merupakan salah satu teknik yang boleh-suai, pantas, dan mantap untuk mengintegrasikan persamaan Schrödinger yang bergantung kepada masa. Di samping itu, derivasi rangka kerja bagi skim pembezaan terhingga dan analisis kestabilan untuk teknik ini telah dibentangkan. Akhir sekali, prestasi skim Crank-Nicolson dianalisa dengan mengira ralat di antara penyelesaian anggaran dan penyelesaian tepat. Didapati bahawa penyelesaian daripada kaedah berangka adalah dan menyamai penyelesaian tepat.

TABLE OF CONTENTS

TITLE		PAGE
	DECLARATION	**iiii**
	DEDICATION	**iv**
	ACKNOWLEDGEMENT	**v**
	ABSTRACT	**vi**
	ABSTRAK	**vii**
	TABLE OF CONTENTS	**viiiiii**
	LIST OF TABLES	**x**
	LIST OF FIGURES	**xi**
	LIST OF ABBREVIATIONS	**xii**
	LIST OF SYMBOLS	**xiiiiii**
	LIST OF APPENDICES	**xiviv**
CHAPTER 1	**INTRODUCTION**	**1**
1.1	Introduction	1
1.2	Research Background	1
1.3	Problem Statement	3
1.4	Research Questions	3
1.5	Objectives of the Research	4
1.6	Significance of the Research	4
1.7	Scope of the Study	5
CHAPTER 2	**LITERATURE REVIEW**	**7**
2.1	Introduction	7
2.2	Description of Schrödinger Equation	7
2.3	Previous Work	10
2.4	Description of Finite Difference Methods	11
2.5	Crank-Nicolson Method and Motivation of Numerical Method	12

CHAPTER 3	**METHODOLOGY**	**15**
3.1	Introduction	15
3.2	Operational Framework of Crank-Nicolson Method	15
3.3	Discretization	19
3.4	Stability Analysis for the Crank-Nicolson Method	22
3.5	Computational Procedure	23
CHAPTER 4	**RESULTS AND DISCUSSIONS**	**29**
4.1	Introduction	29
4.2	Experimental Setting	29
4.3	The Analytical Wave Function	30
4.4	Numerical Results	31
CHAPTER 5	**CONCLUSION AND RECOMMENDATIONS**	**43**
3.1	Introduction	43
5.2	Conclusions	43
5.3	Recommendations	44
REFERENCES		**45**
APPENDIX		**47**

LIST OF TABLES

TABLE NO.	TITLE	PAGE
Table 4.1	The comparisons of the errors in terms of stability conditions and x node.	40

LIST OF FIGURES

FIGURE NO.	TITLE	PAGE
Figure 2.1	The finite potential well.	8
Figure 2.2	The infinite square well.	8
Figure 3.1	A computational molecule for different numerical methods	19
Figure 3.2	Flow chart for the Newton-Raphson method.	24
Figure 4.1	The real part of the wave function.	30
Figure 4.2	The imaginary part of the wave function.	30
Figure 4.3 (a)	Graph of spatial grids vs error for initial time step and $\mathrm{Nx} = 20$.	31
Figure 4.3 (b)	Comparison between exact and numerical solution for initial time step and $\mathrm{Nx} = 20$	32
Figure 4.4 (a)	Graph of spatial grids vs error for $1 \leq t \leq 5$ and $\mathrm{Nx} = 20$.	33
Figure 4.4 (b)	Comparison between exact and numerical solution for $1 \leq t \leq 5$, $\mathrm{Nx} = 20$.	33
Figure 4.5 (a)	Graph of spatial grids vs error for $1 \leq t \leq 5$ and $\mathrm{Nx} = 50$.	34
Figure 4.5 (b)	Comparison between exact and numerical solution for $1 \leq t \leq 5$, $\mathrm{Nx} = 50$.	35
Figure 4.6 (a)	Graph of spatial grids vs error for $1 \leq t \leq 5$ and $\mathrm{Nx} = 100$.	36
Figure 4.6 (b)	Comparison between exact and numerical solution for $1 \leq t \leq 5$, $\mathrm{Nx} = 100$.	36
Figure 4.7	Graph of spatial grids vs error for $t = 1{:}5$ and $\mathrm{Nx} = 150$.	37
Figure 4.8	Graph of spatial grids vs error for $t = 1{:}5$ and $\mathrm{Nx} = 200$.	37
Figure 4.9	Graph of spatial grids vs error for $t = 1{:}5$ and $\mathrm{Nx} = 50$, $r = 0.10$.	39
Figure 4.10	Graph of spatial grids vs error for $t = 1{:}5$ and $\mathrm{Nx} = 100$, $r = 0.10$.	40
Figure 4.11	Graph of spatial grids vs error for $t = 1{:}5$ and $\mathrm{Nx} = 200$, $r = 0.10$.	40

LIST OF ABBREVIATIONS

FDM	-	Finite Difference Method
NLS	-	Nonlinear Schrodinger Equation
ODE	-	Ordinary Differential Equation
PDE	-	Partial Differential Equations
NaN	-	Not a Number
NPDE	-	Nonlinear Partial Differential Equation

LIST OF SYMBOLS

k	-	Temporal step size
h	-	Spatial step size
r	-	Temporal step size/ square of the Spatial step size
λ	-	Arbitrary constant
x	-	Pressure
t	-	Space
r	-	Time

LIST OF APPENDICES

APPENDIX	TITLE	PAGE
Appendix A	Exact solution’s code	43
Appendix B	Pseudo code of Crank-Nicolson	44

CHAPTER 1

INTRODUCTION

1.1 Introduction

Partial differential equations (PDE) are very common in mathematics, physics, and chemistry fields. These equations are pertinent to model and describe a wide range of physical systems or chemical reactions, which depict real-world problems. One of the most prevalent and widely used PDE in the abovementioned fields is the nonlinear Schrödinger equation (NLS). Solving NLS equation gives a wave function that makes it easier to examine the behaviour or performance of a physical system or chemical reaction. Numerous methods are suitable to solve the Schrödinger equation. This research focuses on one of these methods – the Crank-Nicolson method. Therefore, the primary purpose of this research is to determine a numerical solution for the Schrödinger equation using Crank-Nicolson method.

1.2 Research Background

Nonlinear Schrödinger equation is one of the essential mathematical equations used in mathematics, physics, and chemistry fields. The equation is a second order nonlinear differential equation or a partial differential equation. When it is solved, the solution gives a wave function with information about the behaviour of a particle in time and space. In other words, NLS is applied to describe the behaviour of physical phenomena (Okock and Burns, 2015).

Understanding the behaviour of such systems is very important in different aspects of life. This knowledge can be utilized to design systems that are safe and prone to events that are likely to happen in the future and affect the system. For example, the knowledge can be used by engineers to find the best designs and materials for constructing pipelines to be used in areas with high-temperature variations. In such a case, Schrödinger equation can simulate the behaviour of the pipelines when exposed to different changes and establish appropriate measures that should be put into place to enhance the functionality, safety, and durability of the pipelines.

Several experimental studies conducted by different researchers suggested that atomic particles exhibited wave-like properties. As a result of this, it was concluded that the behaviour of atomic particles could be explained using a wave equation, which is a NLS (Barsan, 2015). The first person to write such an equation was Schrödinger. This wave equation became a subject of discussion for many years and it was found that its eigenvalues were equal to the quantum mechanical system's energy levels. The eigenvalues were formulated from Fourier series, which expresses a mathematical function as the sum of infinite sequence of periodic functions(Knyazev and Shcherbakova, 2017). After numerous discussion about the wave equation, it also became accepted for use in probability distribution. The Schrödinger equation started being used to determine acceptable energy levels of quantum mechanical systems and its wave function was used to determine the probability of an atomic particle at a particular position and at a certain time.

The biggest problem of Schrödinger equation was to find its correct solution (the wave function) that had the right amplitudes such that when they were summed by superposition, they gave the correct or anticipated solution. For many years, researchers struggled to develop methods of solving Schrödinger equation (Popelier, 2011). In an attempt to simplify the problem, the system's wave function, which was the solution to the Schrödinger equation, was replaced by an infinite series of wave functions for individual series. Schrödinger discovered that the individual wave functions described the states of individual quantum systems and the amplitudes of these wave functions provided very useful information about the state of the entire quantum system being examined. At first, the Schrödinger equation appeared to be very complex hence the need to find simpler methods of solving it.

Today, there are several analytical and numerical methods that can be applied to solve Schrödinger equation. Numerical are the widely used methods because they are accurate and easy to use. These methods are also suitable for use in numerous computer programs and applications available today. Some of the numerical methods that solve Schrödinger equation include: finite element method, finite difference method, Crank-Nicolson method, Rayleigh-Ritz method, matrix method, Monte Carlo method, and meshless methods, among others.

1.3 Problem Statement

Nonlinear Schrödinger equation is a very essential mathematical equation and it is important to have an accurate and reliable method of solving it. There are several methods that can be used to find the numerical solution for the Schrödinger equation. Each of these methods has a difference accuracy order. If the Schrödinger equation is not solved accurately then finding a solution to the problem, it represents becomes very difficult. In this research, Crank-Nicolson method will be used to solve the Schrödinger equation and results found compared with the exact solutions. This will help to establish the suitability, accuracy and reliability of Crank-Nicolson method in finding numerical solution for the Schrödinger equation.

1.4 Research Questions

The followings are the research questions.

a) How is Crank-Nicolson method used to solve the Schrödinger equation numerically?
b) Is the solution for the Schrödinger equation obtained using Crank-Nicolson method the same as the exact solution?
c) Is Crank-Nicolson method a simple, accurate and reliable method in determining numerical solutions to the Schrödinger equation?

1.5 Objectives of the Research

The followings are the main objectives of this research:

a) To use Crank-Nicolson method and solve the one dimensional (1D) nonlinear Schrödinger equation (NLS) numerically.
b) To conduct error analysis in solving 1D NLS using Crank-Nicolson method.

.

1.6 Significance of the Research

Solving NLS accurately is beneficial in solving NPDE (nonlinear partial differential equation). NLS can be utilized to model and represent various real-life problems or situations. Understanding how to solve this equation can help find solutions to some of the difficulties people experience in their day-to-day activities. However, the understanding of how to solve NLS is more critical for mathematicians, engineers, scientists, and researchers who are obligated to find solutions to societal problems.

The professionals can use the information obtained from the numerical solution of NLS to understand the behaviour and performance of various design components or systems and design components or systems that are more functional, safe, reliable, durable and cost effective. Therefore, the significance of this research is to demonstrate the suitability, accuracy and reliability (explained in chapter three section 3.4) of using Crank-Nicolson method in finding solution for the NLS. This will ascertain if Crank-Nicolson method is suitable, accurate and reliable enough for use in simulating and solving complex and large real problems.

It is worth noting that most of the problems or systems can be modelled or simulated in form of NLS. When this is done, it becomes very easy to understand the problem/system as it is currently and even predicting how it will be in the future. Predicting the future behaviour of a system is very important because it helps to identify suitable actions or decisions that should be made so as to prevent deterioration of the system when it is exposed to certain conditions.

1.7 Scope of the Study

The main focus of this research is on finding numerical solution for 1D NLS using Crank-Nicolson method. The project will find out the numerical solution using Crank-Nicolson method and comparing the solutions obtained with exact solutions of the equations. This will help to establish the suitability, accuracy and reliability of using Crank-Nicolson method in solving Schrödinger equation by Dirichlet boundary conditions.

REFERENCES

Antoine, X., Bao, W. and Besse, C. (2013) 'Computational methods for the dynamics of the nonlinear Schrodinger/Gross-Pitaevskii equations'. doi: 10.1016/j.cpc.2013.07.012.

Barsan, V. (2015) 'Understanding quantum phenomena without solving the Schrödinger equation: The case of the finite square well', *European Journal of Physics*. IOP Publishing, 36(6), p. 65009. doi: 10.1088/0143-0807/36/6/065009.

Besse, C. *et al.* (2019) 'Energy preserving methods for nonlinear Schrödinger equations To cite this version : HAL Id : hal-01951527'.

Boykin, T. B. and Klimeck, G. (2004) 'The discretized Schrödinger equation and simple models for semiconductor quantum wells', *European Journal of Physics*, 25(4), pp. 503–514. doi: 10.1088/0143-0807/25/4/006.

Chapra, C. S. (2006) 'Part One.', in *Applied Numerical Methods with Matlab for engineers and scientists.* Second. McGraw-Hill Higher Education, p. 3.

Choy, Y. Y. *et al.* (2014) 'Crank-Nicolson implicit method for the nonlinear Schrodinger equation with variable coefficient', *AIP Conference Proceedings*, 1605, pp. 76–82. doi: 10.1063/1.4887568.

Doina Cioranescu, Patrizia Donato, M. P. R. (2017) *An Intoduction To Second Order Partial Differential Equations*. First. Singapore: World Scientific Publishing Co. Pte. Ltd.

Doma, S. B. and E.-S. (2016) 'Second Order Partial Differential Equations and their Applications', (December).

Fadugba, S. *et al.* (2013) 'Crank Nicolson Method for Solving Parabolic Partial Differential Equations', *International Journal of Applied Mathematics and Modeling IJA2M*, 1(3), pp. 8–23. Available at: https://www.researchgate.net/publication/2871952030Awww.kindipublication.com.

Farokhi, B. (2012) 'Numerical solution of the two-dimensional nonlinear Schrodinger equation; Homotopy perturbation method', *39th EPS Conference on Plasma Physics 2012, EPS 2012 and the 16th International Congress on Plasma Physics*, 3(October), pp. 1915–1918.

Gilat, A. and Subramaniam, V. (2011) 'Introduction.', in *Numerical Methods, An introduction with Applications using MATLAB.* Second. John Wiley & sons , INC., p. 1.

Knyazev, S. Y. and Shcherbakova, E. E. (2017) 'Method for Numerical Solution of the Stationary Schrödinger Equation', *Russian Physics Journal,* 59(10), pp. 1616–1622. doi: 10.1007/s11182-017-0953-6.

Ma, C., Cao, L. and Lin, Y. (2018) 'Error estimates of Crank-Nicolson Galerkin method for the time-dependent Maxwell-Schrödinger equations under the Lorentz gauge', *IMA Journal of Numerical Analysis*. Oxford University Press, 38(4), pp. 2074–2104. doi: 10.1093/imanum/drx060.

Oishi, C. M. *et al.* (2015) 'Stability analysis of Crank–Nicolson and Euler schemes for time-dependent diffusion equations', *BIT Numerical Mathematics*, 55(2), pp. 487–513. doi: 10.1007/s10543-014-0509-x.

Okock, P. and Burns, T. (2015) 'A Matrix Method of Solving the Schrodinger Equation', (August 2015).

Popelier, P. (2011) *Solving The Schrodinger Equation: Has Everything Been Tried?* First edit. London: Imperial College.

Renn, J. (2013) 'Max Planck Institute for the History of Science', *Writing*, 114.

Roknuzzaman, M. *et al.* (2015) 'Analysis of Rectangular Plate with Opening by Finite Difference Method', *American Journal of Civil Engineering and Architecture, Vol. 3, 2015, Pages 165-173*, 3(5), pp. 165–173. doi: 10.12691/AJCEA-3-5-3.
Science, N. D. of M. (2013) 'Nonlinear schrödinger equation', pp. 1–12.

Szczepankiewicz, W. (2018) 'Time-Independent Schrödinger equation as a straight line equation in Cartesian coordinates', *International Journal of New Technology and Research*, 4(6), pp. 21–24. doi: 10.31871/ijntr.4.6.62.

Trofimov, V. A. and Trykin, E. M. (2018) *Implicit finite-difference schemes, based on the Rosenbrock method, for nonlinear Schrödinger equation with artificial boundary conditions, PLoS ONE*. doi: 10.1371/journal.pone.0206235.

Wani, S. S. and Thakar, S. H. (2013) 'Crank-Nicolson Type Method for Burgers Equation', *International Journal of Applied Physics and Mathematics*, (January), pp. 324–328. doi: 10.7763/ijapm.2013.v3.230.

Wong, B. R. (2009) 'Numerical solution Of the Time-Dependent Schrödinger equation', *AIP Conference Proceedings*, 1150(July 2009), pp. 396–401. doi: 10.1063/1.3192278.