A NUMERICAL STUDY OF SCHRODINGER EQUTION BY DIFFERENTIAL QUADRATURE METHODS

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By

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DECLARATION

I, Ashish Pradhan, hereby declare that the dissertation entitled "A Numerical Study of Schrödinger Equation by Differential Quadrature Methods" is an original work carried out by me under the guidance of Dr. Thoudam Roshan Singh. The contents of this dissertation did not form the basis of any previous degree to me or to the best of my knowledge, and that the dissertation has not been submitted by me for any research degree in any other university/institute. This is submitted to Sikkim University for the award degree of Master of Philosophy in Mathematics.

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A Numerical Study of Schrödinger Equation by Differential Quadrature Methods

Submitted by **Ashish Pradhan** under the supervision of **Dr. Thoudam Roshan Singh** of the Department of MATHEMATICS School of PHYSICAL SCIENCES, Sikkim University, Gangtok, 737102, INDIA

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June, 2018

To my family

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Abstract

The purpose of this work is to test the application of the Localized Differential Quadrature Method to Solitary wave solution problems, in particular for solving the Schrödinger equation. In chapter 1 we begin with an overview of solitary waves, soliton, the Schrödinger equation and introduction to the Differential Quadrature method. In chapter 2 we give an overview of quantum mechanics, derive the cubic Schrödinger equation and discuss the basic conservation laws. Different types of Differential Quadrature methods are discussed in chapter 3 in detail. In chapter 4 the Cubic Schrodinger equation is solved by using Quintic B-Spline based differential quadrature method and Cosine based differential quadrature method. Similarly the coupled Schrodinger equation is solved in chapter 5 by using Quintic B-Spline based differential quadrature method.

CONTENTS

1. Introduction

Most of the physical phenomenon of the universe are governed by different type of waves such as sound waves, water waves etc. In pursue of understanding and unravelling the physical phenomenon of the universe we need to study the waves, the wave equation is an important mathematical tool for the description of waves. By studying these equations and determining the wave functions we can learn about the properties of the waves, properties of a particle. The Schrödinger Equation is one of the most famous and fundamental wave equation.

1.1 Schrödinger Wave Equation

The wave-particle duality was first reflected in Albert Einstein's work, in which he proposed that the energy of a photon is directly proportional to its frequency. Louis de Broglie hypothesized that the wave-particle duality is true for all atomic and sub-atomic particles not only for the photons. He later proved the theory for electrons and showed that the electron forms some kind of standing waves. Erwin Schrödinger learned of de Broglie's work and even before the experimental confirmation, he realized the significance of de Broglie's work and he was so much fascinated that he wrote to Einstein saying, "I have been intensely concerned these days with Louis de Broglie's ingenious theory. It is extraordinarily exciting, but still has some very grave difficulties."

Later, while Schrödinger was giving lecture in a seminar, a scholar asked him why there was no equation to show how de Broglie's waves change with time, as there was for electromagnetic waves, if particles behaves as waves then they should satisfy some sort of wave equation. Schrödinger got to work and in two weeks proposed the three dimensional wave equation,

which he published in 1926. The equation was later named after him. Schrödinger himself describe the equation as follow: “The already mentioned Psi-function is now the means of predicting probability of measurement results. In it is embodied the momentarily attained sum of the theoretically based future expectation, somewhat as laid down in a catalog.” The Schrödinger equation is one of the most important and fundamental equation of the modern physics. The study of this equation plays an exceptional role in modern physics. The Schrödinger equation is a space-time partial differential equation, which describes the form of the probability waves that govern the motion of small particles, and it specifies how these waves are altered by external influences. It has been shown as a model of wide class of physical phenomena such as propagation of optical pulses, waves in water, waves in plasmas, electromagnetic waves etc. In mathematics, the Schrödinger equation and its variants are one of the basic equations that are studied in the field of partial differential equations, and has applications to geometry, to spectral and scattering theory, and to integrable systems. After the discovery the equation has been studied widely by researchers and has been interpreted in various mathematical forms.

1.2 Solitary Waves and Solitons

A solitary wave is a localized wave which maintains its coherence and its visibility through properties of nonlinear hydrodynamics. Solitary waves have finite amplitude and propagate with constant speed and constant shape. Whereas a soliton is a solitary wave packet which propagate at a constant velocity while maintaining its shape. Solitons are caused by a cancellation of nonlinear and dispersive effects in the medium (The term "dispersive effects" refers to a property of certain systems where the speed of the waves varies according to frequency). Solitons are the solutions of scattered class of weakly nonlinear dispersive partial differential equations describing physical systems [1].

Story of solitary waves and solitons begins with John Scott Russell's [2] visionary observation in the year 1834. In the canal of Edinburgh he was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horse when the boat stopped it created a water front (which he called a 'wave of translation') in the canal which started moving with a constant velocity and preserving its shape. He chased it and claimed that the wave was moving with a velocity around 9 miles per hour and the front was one to one and half feet high and about thirty feet in length. He lost the wave after following it for couple of miles in the windings of the canal. For more than a half of the century scientific community was sceptical about this non dispersive water wave. The debate continued till 1895, when two mathematicians Korteweg and de Vries [2] came up with an equation, known as KdV equation, for shallow inviscid fluids based on firm physical arguments. Their mathematical formulation showed the existence of such a wave and put an end to the controversy. Scott Russel tried to produce experimentally this type of waves in his laboratory and made the following important observations [2].

1. They are non-dispersive, i.e. maintain their shapes and size.

2. The velocity of the wave if proportional to the amplitude.

3. They break into smaller ones of with the above properties.

4. Collisions of two or more such waves are like perfect elactic collisions.

After merger the both waves again separate maintaining their original shapes and velocities. The 4^{th} property distinguishes a Soliton from a solitary wave. The later collides inelastically and can lose energy. Solitons are stable bound states in classical and quantum field theories. For the existence of solitons one needs right amount of nonlinearity in the system. A weak nonlinear coupling does not limit the possibility of soliton, i.e. weak coupling does not necessarily mean a weak amplitude for a soliton.

1.3 FPU Recurrence

We consider a linear chain of particles of with equal masses B connected by elastic springs. The linear part of the force with a constant force F gives the harmonic frequencies $\lambda_0 = \sqrt{2\,F/B}$ for all particles.

If we consider the case $B = F = 1$, the nonlinear force (only considering the quadratic case), the equation is given by

$$\ddot{x}_n = (x_{n+1} - 2x_n + x_{n-1}) + \beta[(x_{n+1} - x_n)^2 - (x_n - x_{n-1})^2] \qquad 1.1$$

Where x_n represents the displacement of the nth particle from its original position and β represents the strength of nonlinear interactions between particles. In the case of normal nonlinear interaction mode, the equation of the motion is given by

$$\ddot{W}_k + \lambda_k^2 W_k = \beta \sum_{i,j=1}^{N} m_{ij}\, W_i W_j \qquad 1.2$$

Where m_{ij} is the coefficient of the complicated dependence. Usually in this kind of oscillation, the energy spreads to higher harmonics but after certain oscillation period, the flow of the energy into other modes stops. After that the dynamics reverse and energy flow back into the first mode. In this reverse mechanism the energy is almost same, which implies that there is absence of thermalization [3, 4].

With an increase in the coefficients of nonlinearity the period of a recurrence decreases. The evolution of time does not leads to the energy equipartition, rather implicated the existence of

quasi-modes consisting of a number of linear modes. It is possible to reach numerically the initial state, unless the reversal time is relatively strong.

1.4 Differential Quadrature Method

The Differential Quadrature Method (DQM) is a numerical solution technique for initial and/or boundary value problems. Its ease to apply for getting numerical solutions of partial differential equations when compared with finite element methods makes the method preferable. DQMs was first introduced by Bellman et al. (1971, 1972) [5]. In this method a partial derivative of a function with respect to a coordinate direction is expressed as a linear weighted sum of all the functional values at all grid points along that direction. In 1972, Bellman provided two different methods to determine the weighting coefficients of first order derivative. The first method solves an algebraic equation system. In second method he uses a simple algebraic formulations, where the roots of the Legendre Polynomials are chosen as the coordinates of grid points. Thus, it is difficult to obtain the weighting coefficients. To improve the computation, Quan and Chang (1989) [6] used the Lagrange Interpolated polynomials as test functions and obtained recursive formulae to calculate the weighting coefficients of the first and second order derivatives. Shu [5] and Richards (1990) generalized all the current methods for determination of the weighting coefficients under the analysis of a high order polynomial approximation and the analysis of a linear vector space. The weighting coefficients of the first order derivative are determined by an algebraic formulation however the weighting coefficients of the second and higher order derivatives are determined by a recurrence relationship. The mathematical representation of differential quadrature is given by

$$U_x^{(p)} = \sum_{j=1}^{N} A_{ij}^{(p)} U(x_j), i = 0,1\ldots, N \qquad 1.3$$

Where $U_x^{(p)}$ is the p^{th} order derivative of the function U w.r.t the variable x and $A_{ij}^{(p)}$ are the weighting coefficients of the p^{th} order derivatives. The most important work here is to determine the weighting coefficients which can be done by using function approximation method. There are two techniques to determine the weighting coefficients:

• The first technique to obtain the weighting coefficient is by solving a system of algebraic equations.

• The second technique to obtain weighting coefficient is by using algebraic formulation with grid points in Legendre polynomial.

1.5 Objectives

- To solve the cubic Schrödinger equation and the coupled Schrödinger equation.
- To use the Differential Quadrature Methods as the tool to approximate the above equations.
- To introduce the Quintic B-spline function as the test function, to find the weighting coefficients.
- To compute the two basic conserved quantities.
- Finally, determining the error by comparing the obtained results with the analytical solutions.

2. Schrödinger Equation

2.1 The Duffing Oscillator

The Duffing oscillator is a non-linear differential equation of second-order which represents certain model of damped and driven oscillators. The equation is given by

$$\ddot{x} + \delta\dot{x} + \beta x + \theta x^3 = \sigma Cos(\omega t) \qquad 2.1$$

Where the function $x = x(t)$ represent the displacement at any time t, $\dot{x}$ and $\ddot{x}$ represent the first and second order derivative of x with respect to time t respectively. δ controls the amount of damping, β is the amount of linear stiffness, θ controls the amount of non-linearity in the restoring force, for $\theta = 0$, Duffing equation describes a damped and driven simple harmonic oscillator, σ represent the amplitude of the periodic driving force; if the system is without a driving force, and ω represent the angular frequency of the periodic driving force [7, 8].

The Duffing oscillator differs from the forced and damped harmonic oscillator by the nonlinear $term\ \theta x^3$, which changes the dynamics of the system drastically. The equation represents the motion of a damped oscillator with a more complex potential than in simple harmonic motion.

The Duffing equation is an illustration of a dynamical system that exhibits chaotic activity. However, the Duffing system indicates the jump resonance phenomenon in the frequency response that is a sort of frequency hysteresis characteristic.

The Duffing oscillator represents the mass oscillations attached to a nonlinear spring and a linear damper. The restoring force provided by the nonlinear spring is then $\beta x + \theta x^3$. When $\beta > 0$ and $\theta > 0$, the spring is called a hardening spring. Conversely, if $\theta < 0$ then it is a

softening spring (with $\beta > 0$). Generally, the adjectives hardening and softening are considered with respect to the Duffing equation which depends on the values of β and θ accordingly.

We can reduce the number of parameters in the Duffing equation by two, through scaling. For example we can scale the excursion x and t as $y = x\beta/\sigma$ and $T = t\sqrt{\beta}$. We assume β to be positive, hence we arrive at

$$\ddot{y} + 2\eta\dot{y} + y + \tau y^3 = Cos(\xi T) \qquad 2.2$$

Where $\eta = \frac{\delta}{2\sqrt{\beta}}$, $\tau = \frac{\theta\sigma^2}{\beta^3}$ and $\xi = \frac{\omega}{\sqrt{\beta}}$

The dots indicates the derivatives with respect to T. We note that the solutions to the forced and damped Duffing equation can be described in terms of the three parameters $(\varepsilon, \eta, \xi)$and initial conditions $y(t_0)$ and $\dot{y}(t_0)$.

2.1.1 Undamped Oscillator

Multiplication of $\dot{u}$ on undamped and unforced Duffing equation and integrating we get [7, 8]

$$\frac{1}{2}\dot{x}^2 + \frac{1}{2}\beta x^2 + \frac{1}{4}\theta x^4 = H \qquad 2.3$$

Where H is a constant whose value is determined by the initial conditions $x(0)$ and $\dot{x}(0)$.

We substitute $\dot{x} = y$ and we note that the system is Hamiltonian:

$$\dot{x} = +\frac{\partial H}{\partial y}, \dot{y} = -\frac{\partial H}{\partial x} \qquad 2.4$$

With

$$H = \frac{1}{2}y^2 + \frac{1}{2}\beta x^2 + \frac{1}{4}\theta x^4 \qquad 2.5$$

The solution is bounded for positive value of β and θ.

2.1.2 Damped Oscillator

Similarly as above, for the damped oscillator, we consider

$$\dot{x}\,(\ddot{x} + \delta\dot{x} + \beta x + \theta x^3) = 0$$

$$\Rightarrow \frac{d}{dt}\left(\frac{1}{2}\dot{x}^2 + \frac{1}{2}\beta x^2 + \frac{1}{4}\theta x^4\right) = -\delta\dot{x}^2$$

$$\Rightarrow \frac{dH}{dt} = -\delta\dot{x}^2 \leq 0, \qquad 2.6$$

As $\delta \geq 0$for damping, the damped Duffing oscillator will end up at its stable equilibrium points without forcing. The points of stable and unstable equilibrium are at $\beta x + \theta x^2 = 0$. The equilibrium state is at $x = 0$ if $\beta > 0$and if $\beta < 0$ and $\theta > 0$ the stable equilibria are at

$$x = \sqrt{-\beta/\theta} \quad \text{And} \quad x = -\sqrt{-\beta/\theta}\ .$$

2.2 Perturbation Series Solution

We consider a Duffing oscillator with small cubic nonlinearity and a harmonic driving force. Equation of motion is given by

$$\ddot{x} + 2\sigma\dot{x} + \beta x + \mu x^2 = Fexp\big(i(\omega t + \phi)\big) + CC \qquad 2.7$$

Where, the complex conjugate of the preceding term is given by *CC* [9]. Since the use of complex forces and taking real part of the resulting solution presupposes linearity, therefore it is important to use a real driving force. We assume that μx^3 is small compared to the other terms of the equation (2.5) and look for solutions which are close to the corresponding solutions of the linear equation with $\mu = 0$. Therefore it is natural to expand the solution into a perturbation series with respect to μ

$$x(t) = \sum_{i=0}^{\infty} x_i(t)\mu^i \qquad 2.8$$

Substituting the series (2.8) into the equation of the motion (2.7) and equating terms with the same powers of μ gives a hierarchy of linear and inhomogeneous equations which can be explicitly solved. This can be shown by induction that all functions with frequency ω. Therefore they can be expanded into Fourier series, as follow [10]

$$x_n(t) = \sum_{m\in\mathbb{Z}} x_{nm} e^{im\omega t} \qquad 2.9$$

Since $x(t)$ is a real function we can write $x_{n,-m} = \bar{x}_{nm}$ and we only need to consider non-negative n, m.

By use of the computer algebra software it is possible to calculate a certain number of terms of the perturbation series, it is obvious that they will become more and more complex. We will only explicitly calculate the first few terms in order to see the underlying principle.

$\mu^0\ terms$:

It is sufficient to re-derive the result of the linear problem, which gives,

$$x_0(t) = x_{01} e^{i\omega t} + CC \quad , \qquad 2.10a$$

$$x_{01} = h(\omega) F e^{i\emptyset} \quad , \qquad 2.10b$$

$$h(\omega) = \frac{1}{\beta - \omega^2 + 2i\sigma\omega} \qquad 2.10c$$

$\mu^1\ terms$:

The cubic terms gives

$$\mu(x_0 + x_1\mu + \cdots)^3 = \mu x_0^3 + \mathcal{O}(\mu^2) = \mu\left(x_{01}^3 e^{3i\omega t} + 3x_{01}^2 - x_{01} e^{i\omega t} + \mathrm{CC}\right) + \mathcal{O}(\mu^2). \qquad 2.11$$

Since the driving force is $\mathcal{O}(\mu^0)$, the $\mathcal{O}(\mu^1)$ of (2.7) are

$$\ddot{x}_1 + 2\sigma\dot{x}_1 + \beta x_1 = -x_0^3 = -\left(x_{01}^3 e^{3i\omega t} + 3x_{01}^2\overline{x_{01}}e^{i\omega t} + CC\right),$$

$$\frac{1}{h(\omega)}x_{11} = -3F^3 e^{i\emptyset}h^2(\omega)\overline{h(\omega)} \quad ,$$

$$x_{11} = -3F^3 e^{i\emptyset}h^2(\omega)\overline{h(\omega)} \quad , \qquad 2.12a - e$$

$$\frac{1}{h(3\omega)}x_{13} = (-Fe^{i\emptyset}h^2(\omega))^2 \quad ,$$

$$x_{13} = (-F^3 e^{3i\emptyset}h^3(\omega))h(3\omega) \quad .$$

In equation $(2.12a)$ we note that the cube of the solution in $\mathcal{O}(\mu^0)$ approximation acts as a driving force for the next order approximation. Since x_0^3 contains the frequencies $\omega$and 3ω, implies that $x_1(t)$ will contain terms with these frequencies. Both terms are proportional to F^3, F being essentially the amplitude of the driving force. Therefore the nonlinear term μu^3produces a correction to the linear response of the oscillator with the same frequency as well as a correction with triple frequency (third harmonic generation) in the lowest order. Both terms could be split into a relative amplitude and a phase shift part, similar but more complicated than in the linear theory.

$\mu^2\ terms$:

We conclude similar as above

$$\ddot{x}_2 + 2\sigma\dot{x}_2 + \beta x_2 = -3x_0^2 x_1 = -3\left(x_{01}e^{i\omega t} + CC\right)^2 + \left(x_{11}e^{i\omega t} + x_{13}e^{3i\omega t} + CC\right)$$

$$\frac{1}{h(5\omega)}x_{25} = -3x_{01}^2 x_{13}$$

$$x_{25} = 35e^{5i\emptyset}h^5(\omega))h(3\omega)h(5\omega) \qquad 2.13$$

…….

It is not necessary to give more terms. We can note that the $\mathcal{O}(\mu^0)$terms will contain the frequencies $\omega, 3\omega, 5\omega$ and the correction will be of order F^5. We emphasize the above findings in order not to generate the wrong impression that a cubic nonlinearity would at most produce

3ω terms proportional to F^5. It seems fairly clear that the higher order corrections conclude all odd multiples of 3ω and odd powers of F, on the contrary.

2.3 Derivation of Schrödinger Equation

The Lorentz model is a simple mechanical model to describe the linear response of matter to electromagnetic waves. The electrons in a piece of matter (insulator) are considered as classical harmonical damped oscillators subject to the driving force of the electromagnetic field. The resulting motion (oscillating) of the electrons produces a polarization density A which determines the dielectric displacement S and the dielectric function $\tau(\omega)$. A linear wave equation is derived from this. We will extend this model to a nonlinear oscillator one with a cubic nonlinearity μx^3(Duffing oscillator) and we will consider the resulting correction of lowest order to the linear wave equation. We will call this model the "Duffing-Lorentz model". We first consider the microscopic Maxwell equations

$$curl\ E + \frac{\partial}{\partial t}B = 0, \qquad divS = 0, \tag{2.14a}$$

$$curl\ H - \frac{\partial}{\partial t}S = 0, \qquad divB = 0, \tag{2.14b}$$

And we assume the following results

$$B = \gamma_0 H\ , \tag{2.15a}$$

$$B = \tau_0 E + A(E)\ . \tag{2.15b}$$

Taking the curl of equation $(2.14a)$ and using $(2.14b)$, $(2.15a)$ and $(2.15b)$ gives

$$curl\ curl\ E\ = \nabla(\nabla.E - \nabla E)$$
$$= \frac{-\partial}{\partial t}\nabla \times B$$

$$= -\gamma_0 \frac{\partial^2}{\partial t^2} S$$

$$= -\gamma_0(\tau_0 \ddot{E} + \ddot{A}) \,. \qquad 2.16$$

Next we take the special situation where the fields E and A points into $z - direction$ and depends only on x, y, z. Let us consider

$$E = \begin{pmatrix} 0 \\ 0 \\ E(x,y,z) \end{pmatrix}, \qquad A = \begin{pmatrix} 0 \\ 0 \\ A(x,y,z) \end{pmatrix} \qquad 2.17$$

It follows that $\Delta . E = 0$ and

$$E = \begin{pmatrix} 0 \\ 0 \\ E_{xx} + E_{yy} \end{pmatrix} \qquad 2.18$$

Hence equation (2.16) reduces to the scalar equation

$$E_{xx} + E_{yy} = \tau_0 \ddot{E} + \ddot{A}. \qquad 2.19$$

For an electron with mass M and charge Q, the Duffing-Lorentz model is given by

$$M\ddot{z} + 2\Gamma\dot{z} + M\beta z + \Lambda z^3 = Qe^{i\omega t}\tilde{E} + CC \qquad 2.20$$

We divide equation (2.20) by mass of the electron *M* and introduce a new parameters and we get,

$$\ddot{z} + 2\sigma\dot{z} + \beta z + \mu z^3 = Fe^{i\emptyset}e^{i\omega t} + CC \qquad 2.21$$

The nonlinear response to the harmonic driving force referring to the equations $2.12a - 2.12e$ will be

$$z(t) = (Fe^{i\emptyset}h(\omega)e^{i\omega t} - 3\mu F^3 e^{i\emptyset}h^2(\omega) - h(\omega)e^{i\omega t} -$$

$$\mu F^3 e^{3i\emptyset}h^3(\omega)h(3\omega)e^{3i\omega t}) + CC + O(\mu^2) \qquad 2.22$$

Which yields an electric dipole density

$$A = QKz(t), \qquad 2.23$$

Where *K* represent the constant electric density.

We consider the following Fourier components of E and A in the approximation with the frequencies ω and 3ω therefore we have

$$E = (E_1(x,y)e^{i\omega t} + E_3(x,y)e^{3i\omega t}) + CC \quad 2.24a$$

$$A = (A_1(x,y)e^{i\omega t} + A_3(x,y)e^{3i\omega t}) + CC \quad 2.24b$$

Hence equation (2.18) assumes the form

$$E_{1xx} + E_{1yy} = \gamma_0(\tau_0 E_1 + A_1)(-\omega^2) \quad 2.25a$$

$$E_{3xx} + E_{3yy} = \gamma_0(\tau_0 E_3 + A_3)(-9\omega^2) \quad 2.25b$$

Using $\frac{QE_1}{M} = Fe^{i\emptyset}$ and equations (2.22), (2.23) we obtain the following equations

$$A_1 = QK(\tfrac{QE_1}{M}h(\omega) - 3\mu(\tfrac{Q}{M})^3 E_1|E_1|^2 h^2(\omega) - h(\omega)) \quad 2.26a$$

$$\equiv \frac{1}{\gamma_0}(n_1(\omega)E_1 + n_1(\omega)E_1|E_1|^2) \quad 2.26b$$

$$A_3 = -\mu(\tfrac{QE_1}{M})^3 h^3(\omega)h(3\omega) + \tfrac{QE_3}{M}h(3\omega) \quad 2.26c$$

We substitute equation $(2.26b)$ into $(2.25a)$ and we obtain the nonlinear wave equation

$$E_{1xx} + E_{1yy} = -\omega^2\left(\left(\tau_0\gamma_0 + \eta_1(\omega)\right)E_1 - \eta_3(\omega)E_1|E_1|^2\right). \quad 2.27$$

We substitute its solution into equation (2.26b) then equation (2.25a) assumes a linear inhomogeneous wave equation for the 3ω component of the electromagnetic wave. Coming back to the equation (2.27) we consider the ansatz of a modulated plane wave in $x - direction$ with an amplitude envelope

$$E_1(x,y) = \psi(x,y)\exp(-irx) \quad 2.28a$$

And we obtain

$$E_{1x} = (\psi_x - \mathrm{ir}\psi)\exp(-irx)\,, \quad 2.28b$$

$$E_{1xx} = (\psi_{xx} - 2\mathrm{ir}\psi_x - r^2\psi)\exp(-irx)\ , \qquad 2.28c$$

$$E_{1xx} = \psi_{xx}\exp(-irx) \qquad 2.28d$$

Hence from equation (2.27) we have

$$\left(\psi_{xx} + \psi_{yy} - 2\mathrm{ir}\psi_x - r^2\psi\right)\exp(-irx) = -\omega^2\left(\left(\tau_0\gamma_0 + \eta_1(\omega)\right)\psi\exp(-irx)\right) - \omega^2\eta_3(\omega)\psi|\psi|^2\exp(-irx) \qquad 2.29$$

Using the "thin beam approximation"

$$\psi_{xx} \ll \psi_{yy} \qquad 2.30$$

And

$$\omega^2 = \tau_0\gamma_0 r^2 \qquad 2.31$$

We have the wave equation

$$-2ir\psi_x + \psi_{yy} + \omega^2\eta_1(\omega)\psi + \omega^2\eta_3(\omega)|\psi|^2\psi = 0 \qquad 2.32$$

Using the transformation

$$\phi = \psi\exp(-icx)\ , \qquad 2.33$$

And putting $2rc = \omega^2\eta_1(\omega)$. We made the $\omega^2\eta_1,(\omega)\psi$ term vanish and we arrived at a cubic Schrödinger equation of the following form

$$-2ir\phi_x + \phi_{yy} + \omega^2\eta_3(\omega)|\phi|^2\phi = 0 \qquad 2.34$$

Equation (2.34) is equivalent to the standard form of the cubic Schrödinger equation (CSE) which is given by

$$-i\phi_t + \frac{1}{2}\phi_{xx} + \xi|\phi|^2\phi = 0 \qquad 2.35$$

Here we note that these transformations assumes that $\eta_1(\omega)$ and $\eta_3(\omega)$ are real functions, which is only approximately satisfied if the damping coefficient σ of the Duffing Lorentz model is neglected. The above assumption is a consistent one. In the following subsections we

will go through the energy conservation law of the cubic Schrödinger Equation, which will be only valid if we neglect the dissipative effects.

2.4 Conservation Laws

The Cubic Schrödinger Equation (CSE) possess very vital property that is, infinite number of conserved quantities. This property leads to interpreting the CSE as an infinite dimensional integrable Hamiltonian systems. We consider the first three conservation laws of the CSE which is confirmed by elementary calculations.

We let the Cubic Schrödinger Equation in the following form

$$\psi_t = \frac{i}{2}\psi_{xx} + i\xi\bar{\psi}\psi^2 = 0\ , \qquad 2.36$$

And the complex conjugate of the CSE in the form

$$\bar{\psi}_t = -\frac{i}{2}\bar{\psi}_{xx} - i\xi\psi\bar{\psi}^2 = 0\ , \qquad 2.37$$

We use the integration by parts repeatedly where the boundary term vanish always due to the boundary conditions for $x \to \pm\infty$. The scalar product of wave functions is given by (referring quantum mechanics)

$$\langle\varphi|\psi\rangle \equiv \int \overline{\varphi(x)}\psi(x)dx. \qquad 2.38$$

We consider $\langle\psi|\psi\rangle$, the first conserved quantity. This is the total probability (=1) which should be considered in the course of time in the quantum mechanics ($\xi = 0$). When the dissipative effects are neglected, $\langle\psi|\psi\rangle$ is proportional to the field energy and its conservation is plausible in the context of nonlinear optics.

To prove

$$\frac{d}{dt}\langle\psi|\psi\rangle = 0 \qquad 2.37a$$

We have

$$\frac{d}{dt}\langle\psi|\psi\rangle = \langle\psi_t|\psi\rangle + \langle\psi|\psi_t\rangle \qquad 2.37b$$

$$= \left\langle \frac{i}{2}\psi_{xx} + i\xi|\psi|^2\psi_t \middle| \psi \right\rangle + \langle\psi|\psi_t\rangle + \left\langle \psi \middle| \frac{i}{2}\psi_{xx} + i\xi|\psi|^2\psi \right\rangle \qquad 2.37c$$

$$= -\frac{i}{2}\left(\int \overline{\psi_{xx}}\,\psi dx - \int \bar{\psi}\psi_{xx}dx\right) + \xi\left(\int - |\bar{\psi}|\,|\psi|^2\,\psi dx + \int\int i\,|\bar{\psi}|\,|\psi|^2\,\psi dx\right) \qquad 2.37d$$

Integrating (2.37d) by parts we conclude,

$$= -\frac{i}{2}\left(-\int \overline{\psi_x}\,\psi_x dx + \int \bar{\psi}\psi_x dx\right) = 0 \qquad 2.37e$$

The expectation value of momentum $\langle\psi|\mathbb{P}|\psi\rangle = \frac{\hbar}{i}\langle\psi|\psi\rangle$ would be conserved in quantum mechanics. Hence we have

$$\frac{d}{dt}\int \psi\overline{\psi_x} = 0\,, \qquad 2.38$$

For the solution of the CSE.

To prove equation (2.38) we consider the following;

$$\frac{d}{dt}\int \psi\overline{\psi_x} = -\int \overline{\psi_x}\,\psi_t dx + \int \overline{\psi_{xt}}\psi \qquad 2.39a$$

$$= -i\int\left(-\frac{1}{2}\psi_x\overline{\psi_{xx}} + \xi\bar{\psi}\psi^2\overline{\psi_x} + \frac{1}{2}\overline{\psi_{xx}}\psi_x + \xi\psi\overline{\psi_x}^2\psi_x\right)dx \qquad 2.39b$$

$$= \frac{i\xi}{2}\int(\psi^2\bar{\psi}^2)_x dx = 0 \qquad 2.39c$$

Which completes the proof of (2.38).

We conclude from the equation (2.38) that the suitable defined centre of mass of the wave packet moves with uniform velocity as in quantum mechanics.

The second conserved quantity in analogy with quantum mechanics is the total kinetic energy expectation value $\langle\psi|\mathbb{P}^2|\psi\rangle$. However in case $\xi \neq 0$ we have add a bi-quadratic term to obtain a conserved quantity:

$$\frac{d}{dt}\int\left(\psi\overline{\psi_x}-\ \xi\psi\overline{\psi_x}^2\right)dx = i\int(\psi_{tx}\overline{\psi_x}-2\xi\psi\bar{\psi}^2\psi_t-\xi\psi^2\overline{\psi\psi_x})dx \qquad 2.40a$$

$$= i\int\left\{\left(\frac{1}{2}\psi_{xxx}+\xi(\bar{\psi}\psi^2)_x\right)\overline{\psi_x}-\left(\frac{1}{2}\overline{\psi_{xxx}}+\xi(\psi\bar{\psi}^2)_x\right)\psi_x-\right.$$
$$\left.2\xi\left(\left(\frac{1}{2}\psi_{xx}+\xi\bar{\psi}\psi^2\right)\psi\overline{\psi_x}^2-\left(\frac{1}{2}\overline{\psi_{xx}}+\xi\psi\overline{\psi_x}^2\right)\bar{\psi}\psi^2\right)dx\right\}$$

2.40b

Integrating (2.40b) by parts the 8 terms cancel pairwise in accordance with the powers of ξ. Hence we have

$$\frac{d}{dt}\int\left(\psi\overline{\psi_x}-\ \xi\psi\overline{\psi_x}^2\right)dx = 0 \qquad 2.40c$$

2.5 Solitary Wave Solution of the Schrödinger Equation

There exist a special class of wave equations which support soliton solutions in different physical system. Particularly, the study of soliton propagation in optical fibre. The soliton pulses are used as the information carriers (elementary bits) to transmit digital signals over long distances. To obtain these special solutions of the cubic Schrödinger Equation (CSE) we insert the ansatz

$$\psi(x,t) = \Psi(x)e^{i\beta t}\ ,\quad \beta\in\mathbb{R} \qquad 2.41a$$

Into the CSE (2.35), and we get

$$-\beta\Psi+\frac{1}{2}\Psi_{xx}+\xi\Psi^3 = 0\,. \qquad 2.41b$$

In the next step, we multiply eq. (2.41b) by $4\Psi_x$ and integrate over x in equivalence with the treatment of one-dimensional equations.

We get,

$$\Psi_x^2-2\beta\Psi^2+\xi\Psi^4 = C\,. \qquad 2.41c$$

On solving equation (2.41a) for Ψ_x and applying separation of variables we arrive at an elliptical integral

$$\int \frac{d\Psi}{\sqrt{C-\xi\Psi^4+\beta\Psi^2}} = \int dx \qquad 2.41d$$

We obtain periodic solutions for $\beta, \xi > 0, C < 0$, and soliton solution for $\beta, \xi > 0, C = 0$.

We perform the transformation $\Psi(x) = g^{-1}(x)$, instead of solving the integral equation (2.41d). Performing the transformation $\Psi_x = -g^{-2}g_x$ in the equation (2.41c),

We get

$$g^{-4}g_x^2 - 2\beta g^{-2} + \xi g^{-4} = 0. \qquad 2.41e$$

Again multiplying (2.41e) with g^4, differentiating it with respect x and then dividing the resultant with $2g_x$ we get the following,

$$g_x^2 - 2\beta g^2 + \xi = 0 \qquad 2.42a$$

$$2g_x g_{xx} - g g_x = 0 \qquad 2.42b$$

$$g_{xx} - 2\beta g = 0. \qquad 2.42c$$

The general solution of the equation (2.42c) satisfying the boundary conditions $\beta, \xi > 0, L \leq 0$ is given by

$$g(x) = A\, Cosh\left(\sqrt{2\beta(x - x_0)}\right). \qquad 2.42d$$

Without loss of generality we let $x_0 = 0$. We can do that since the CSE is invariant with respect to x-translations. The next task we have is to check whether the equation (2.42d) satisfies equation (2.42a), since by differentiation of a differential equation we might have enlarged the set of solitons.

Applying

$$g_x = A\sqrt{2\beta\, Sinh(\sqrt{2\beta x})}\,, \qquad 2.43a$$

We obtain

$$-g_x^2 + 2\beta g^2 = 2\beta A^2[Cosh^2(\sqrt{2\beta x}) - Sinh^2(\sqrt{2\beta x})] = 2\beta A^2 = \xi. \quad 2.43b$$

Which implies that the parameters A, β, ξ cannot be chosen independently and have to satisfy

$$A = \sqrt{\frac{\xi}{2\beta}} \quad 2.44a$$

Hence we invert the above transformation and obtain

$$\psi(x) = \sqrt{\frac{2\beta}{\xi}} Sech(\sqrt{2\beta x}\,) e^{i\beta t}\,. \quad 2.44b$$

Lastly we apply the Galileo transformation to equation (2.44b) and obtain

$$\phi(x,t) = \sqrt{\frac{2\beta}{\xi}} exp\left(i\left(\beta - \frac{1}{2}V^2\right)t + iVx\right) Sech(\sqrt{2\alpha(x - Vt)})\,. \quad 2.44c$$

Equation (2.44c) represents a soliton moving with velocity V in x-direction without changing its form. The amplitude of the soliton is inversely proportional to its width and the distance d between the two points of inflection of the soliton profile is given by

$$d = \sqrt{\frac{2}{\beta}} \log(\sqrt{2} + 1)\,.$$

2.6 Summary of Literature Review

Over the years people have solved the Schrödinger equations using both the analytical and numerical methods. The need for solving the Schrödinger equation numerically can arise in the description of nuclear motion in molecules in the Born-Oppenheimer approximation or in the description of atoms and molecules in self-consistent field approximations.

First the Schrödinger equation was solved with finite differences and a basic propagator in time, and it was then concluded that this method is far too slow and computationally heavy for its use to be justified for this type of problem. In the year 1982 M. D. Feit, J. A. Fleck, JR., and

A. Steiger [11] have provided the Solution of the Schrödinger Equation by a Spectral Method. In this method a new computational method for determining the eigenvalues and Eigen functions of the Schrödinger equation is described. Conventional methods of solving this kind of problem rely on diagonalization of a Hamiltonian matrix or iterative numerical solutions of a time independent wave equation. The new method, in contrast, is based on the spectral properties of solutions to the time-dependent Schrödinger equation. The method requires the computation of a correlation function $<\Psi(r,O)|\ \Psi\ (r,$ t$)>$ from a numerical solution $\Psi\ (r,t)$. Fourier analysis of this correlation function reveals a set of resonant peaks that correspond to the stationary states of the system. Analysis of the location of these peaks reveals the eigenvalues with high accuracy. Additional Fourier transforms of $\Psi\ (r,t)$ with respect to time generate the Eigen functions. Delfour, Fortin, and Payre [12] has also presented a finite difference scheme for solving a non-linear Schrödinger Equation with a Linear Damping term the scheme is shown to give numerical solutions which are in good agreement with analytical solutions for cases in which the damping coefficient v is zero. However, when $v \# 0$, the numerical solutions have sawteeth oscillations (with wavelengths of the order of the mesh spacing) superimposed on the smooth wave solutions. These sawteeth are caused by the incorrect discretization of the damping term in equation.

One of the most significant work has been done by Uri Peskin, Ronnie Kosloff, and Nimrod Moiseyev[13] who have solved the Schrödinger equations by (t,t') method: The use of global polynomial propagators for time dependent Hamiltonians. The crude methods of time propagation were unbalanced with respect to the very high quality of the spatial representation. It was the introduction of the Chebyshev polynomial expansion of the evolution operator which first created a balanced method where both the spatial representation and the evolution operator possessed exponential convergence. The method gains its optimal efficiency for very high order

polynomial expansions. Polynomial orders of a few thousand terms are not uncommon in current applications. For encounters described by a stationary Hamiltonian the extreme accuracy and stability of the Chebyshev expansion have been found to be superior to other propagation techniques. For explicitly time dependent problems the construction of the propagator is more involved due to the problem of time ordering. The customary solution to the problem is to segment the propagation into small intervals for which the time variation of the Hamiltonian is small. The short time intervals mean that the Chebyshev expansion is far from optimal. Therefore new methods for propagation of explicitly time dependent problems have been developed. These methods have been based on short iterative polynomial expansions and the use of the Magnus series to overcome the time ordering problem. The method has been found satisfactory but could not reach the high degree of accuracy and efficiency of the Chebyshev expansion. In particular that any segmented propagation scheme is bound to accumulate errors. In a very non-conventional approach S.R.Kiyegar , G. Jayaraman and V. Balasubramanian [14] has given the Variable Mesh Difference Schemes Solving a Nonlinear Schrödinger Equation with a Linear Damping Term In the variable mesh scheme, the spatial discretization is done in a non-uniform manner with the mesh size refined at the region of large changes. Variable mesh schemes proposed by Jain for solving singular perturbation boundary value problems are extended. D. Kosloff [15] has provided a Fourier method solution for the time dependent Schrödinger equation, the method is based on discretizing space and time on a grid, and using the Fourier method to produce both spatial derivatives, and second order differencing for time derivatives. The method conserves norm and energy, and preserves quantum mechanical commutation relations. One and two dimensional examples, where a comparison to analytic results is possible, are investigated. Jiten C. Kalitaa, Puneet Chhabrab, Sudhanshu Kumarb [16] have provided a semi-discrete higher order compact scheme for the unsteady two-dimensional Schrödinger equation In this study, an implicit semi-discrete higher

order compact (HOC) scheme, with an averaged time discretization, has been presented for the numerical solution of unsteady two-dimensional(2D) Schrödinger equation. The scheme is second order accurate in time and fourth order accurate in space. The results of numerical experiments are presented, and are compared with analytical solutions and well established numerical results of some other finite difference schemes. In all cases, the present scheme produces highly accurate results with much better computational efficiency. In another finite difference scheme Maike Schulte [17] has discuss and analyse the results on open boundary conditions for the two-dimensional time-dependent Schrödinger equation. In his work he has derived a new mathematical models for the simulation of novel electronic devices of nanoscale dimensions. Within these models it is possible to study the electron flow through devices and their operations like the switching behaviour between on- and off states. In practice, devices consist of an "active region" (often having a complicated geometry) which is connected to leads or contact regions. Compared to the domain of interest, these leads are so long that they are usually modelled as infinitely long. For numerical purposes it is hence necessary to reduce the computational domain of the simulation model to a small region around the domain of interest – however, without changing the simulation results. Hence we need to use artificial boundary conditions at the cut-offs of the computational domain. These boundary conditions are called transparent, if the solution on the restricted area with the new boundary conditions coincides with the solution on the unbounded domain (i.e. the channel). The main courtesy of this work is the discretization of such artificial boundary conditions in conjunction with various finite difference schemes for the Schrödinger equations.

In a numerical method for two-dimensional Schrödinger equation using collocation and radial basis functions provided by Mehdi Dehghan, Ali Shokri[18], they have proposed a scheme for the solution of the two-dimensional Schrödinger equation using collocation points and approximated the solution using multiquadrics (MQ) and the Thin Plate Splines (TPS) Radial

Basis Function (RBF). The scheme works in a similar fashion as finite-difference methods Mohandas pilai, Joshua Goglio and Thad g. Walker [19] a case in point is the solution of boundary value problems for the one-dimensional Schrödinger equation. One typically starts at one boundary with an assumed value for the energy, then integrates to the other boundary where the boundary conditions are tested. A new guess for the energy is generated, and the process is repeated until the desired level of accuracy is obtained .Using the Numerov method, the numerical integration can be done with relatively high accuracy even with large step sizes .Though straightforward, this process is tedious to program when one needs to solve for a large number of Eigen states. Wang, and Jiang [20] proposed a numerical scheme to solve the two-dimensional time-dependent Schrödinger equation using the method of particular solution and radial basis function (RBF). In this paper they have develop the multiquadrics (MQ) and the thin plate splines (TPS) (m=3) radial basis function in the MPS. The scheme is similar to finite- difference methods. The time dependent Schrödinger equation have been solved by Diwaker, Bandhan Panda, Aniruddha Chakraborty [21] they have focused on the exact solution of the time dependent Schrödinger equation involving two potentials coupled by a time dependent Dirac Delta function potential. The problem involving the partial differential equations in two variables have been reduced to a single integral equation in Laplace domain and by knowing the wave function at the origin they have derive the wave function everywhere. One of the most relevant work to our work are done by Korkmaz and Idris [34, 35]. They have solved a non-linear Schrödinger equation (NLSE), using two different differential Quadrature methods namely Lagrange based differential quadrature method and Cosine expansion based differential quadrature method. In Lagrange based differential quadrature method they have used the Chebyshev collocation points as the grid points and solved the equation first in the domain [-1, 1] and generalised the solution in an arbitrary domain by using a transformation.

After solving the equation for four different initial conditions they have estimated the error L_2 and L_∞ by using the known analytical solutions.

The computational methods are very efficient schemes to solve the time-dependent Schrödinger equation. But using such methods, gives out unwanted reflections at the boundaries that necessarily constrains the computation area. To minimize these reflections Christoph Wachter [24] has introduced absorbing boundary conditions and has solved the time dependent Schrödinger equation with the Crank-Nicolson method with absorbing boundary conditions. He has examined the effectiveness of the absorbing boundary conditions, as well as calculating transmission coefficients for various shapes of potential barriers.

3. Differential Quadrature Methods (DQMs)

The different types of differential quadrature methods and the corresponding recurrence formulas for determining the weighting coefficients are discussed in this chapter.

3.1 Lagrange Polynomial Based Differential Quadrature (PDQM)

In this method the Lagrange interpolation polynomials are used as base functions, let the set of Lagrange interpolation polynomial be

$$r_k(x) = \frac{M(x)}{(x-x_k)M^1 x_k} \quad , k = 0,1,2, \dots , N \tag{3.1}$$

Where,

$$M(x) = \prod_{i=0}^{N}(x - x_i)$$

And

$$M^{(1)}(x_k) = \prod_{i=0,i\neq k}^{N}(x_i - x_k)$$

constitute an $N + 1$ dimensional vector space and used as the test function for determining the weighting coefficients. After some computation and applying differential quadrature approximation given by Shu [5], the weighting coefficients of the first order derivatives are given as follows

$$A_{ij} = \frac{M^{(1)}(x_i)}{(x_i - x_j)M^{(1)}(x_i)} \tag{3.2}$$

For determining the diagonal weighting coefficients, the test function $r_k(x) = 1$ is chosen from the set of test functions $r_k(x) = x^k \ , k = 0,1,2, \dots , N$

$$\sum_{j=1}^{N} A_{ij} = 0 \qquad or \qquad A_{ii} = -\sum_{j=1,j\neq i}^{N} A_{ij} \quad , i = j \tag{3.3}$$

Weighting coefficients for the second order derivatives can be obtained by the Shu [5] general formula as follows:

$$B_{ij} = 2A_{ij}\left(A_{ij} - \frac{1}{(x_i - x_j)}\right) \quad , i \neq j \tag{3.4}$$

And

$$\sum_{j=1}^{N} B_{ij} = 0 \qquad or \qquad B_{ii} = -\sum_{j=1, j\neq i}^{N} B_{ij} \quad , i = j \tag{3.5}$$

The Recurrence formulas for the weighting coefficients of the higher order derivatives are given as

$$W_{ij} = n\left(W_{ij}^{(n-1)} A_{ij} - \frac{W_{ij}^{n-1}}{x_i - x_j}\right) \quad , i \neq j \, , n = 2,3, \dots , N-1 \tag{3.6}$$

And

$$\sum_{j=1}^{N} W_{ij}^{(n)} = 0 \qquad or \qquad W_{ii}{}^{(n)} = -\sum_{j=1, j\neq i}^{N} W_{ij}^{n} \quad , i = j \tag{3.7}$$

It should be mentioned that, when the problem domain is large the value of $\frac{M^{(1)}(x_i)}{(x_i - x_j)M^{(1)}(x_i)}$ in (3.2) may exceed the computation limits of the computer. So the usage of the uniform grids is not practical for all problems with differential quadrature method based on the Lagrange polynomials. Also Polynomial based Differential Quadrature method is of higher accuracy but poor stability. The high accuracy can be achieved by using more grid points. However, larger grid points unavoidably lead to instability of the results.

3.2 Fourier Expansion Based Differential Quadrature (FDQM)

In this method the Fourier series expansion is used as the base function for the approximation of the function $g(x)$ which is given as

$$g(x) = c_0 + \sum_{k=0}^{\frac{N}{2}} (c_k Cos(kx) + d_k Sin(kx)) \tag{3.8}$$

Here $g(x)$ constitute a $(N+1)$ dimensional vector space. There are two typical sets of base vectors which are used in the formulation of the Fourier Expansion Based Differential Quadrature (FDQ),

$$1, Cosx, Sinx, Cos2x, Sin2x, \ldots\ldots, Cos\left(\frac{Nx}{2}\right), Sin\left(\frac{Nx}{2}\right) \qquad 3.9$$

And

$$s_k(x) = \frac{S(x)}{q(x_k)Sin\frac{x-x_k}{2}} \ , \ k = 0,1,2, \ldots., N \qquad 3.10$$

Where,

$$S(x) = \prod_{k=0}^{N} Sin\frac{x-x_k}{2}$$

$$q(x_i) = \prod_{k=0,k\neq i}^{N} Sin\frac{x_i-x_k}{2}$$

Now after some computation and using eq. (1.3), the weighting coefficients of the first order derivative are given as

$$A_{ij} = \frac{q(x_i)}{2q(x_i)\frac{x_i-x_k}{2}} \quad , j \neq i \qquad 3.11$$

Using the first set of base vectors (3.9), we get

$$\sum_{j=1}^{N} A_{ij} = 0 \quad or \quad A_{ii} = -\sum_{j=1,j\neq i}^{N} A_{ij} \quad , i = j \qquad 3.12$$

And the weighting coefficients of the second order are given by

$$B_{ij} = A_{ij}\left(2A_{ij} - Cot\frac{(x_i-x_j)}{2}\right) \quad , \ i \neq j \qquad 3.13$$

and

$$\sum_{j=1}^{N} B_{ij} = 0 \qquad or \qquad B_{ii} = -\sum_{j=1, j\neq i}^{N} B_{ij} \quad , i = j \tag{3.14}$$

3.3 Sine Expansion Based Differential Quadrature (SDQM)

Here we consider an odd function $g(x)$. Let the Fourier series expansion is used for the approximation of the function $g(x)$ which is of the following form

$$g(x) = \sum_{k=1}^{N} d_k Cos(kx) \tag{3.15}$$

There are two sets of base vectors in a $N+1$ linear vector space, which are used to determine the Sine Expansion Based Differential Quadrature (SDQM)

$$S_k(x) = Sin(kx)\,,\ k = 1,2,\dots,N \tag{3.16}$$

And

$$S_k(x) = \frac{SinC_k(x)}{Sinx_k} \tag{3.17}$$

Where,

$$C_k(x) = \frac{C(x)}{P(x_i)(Sinx - Sinx_i)}$$

Where,

$$C(x) = \prod_{i=1}^{N} (Sinx - Sinx_i)$$

$$P(x_i) = \prod_{k=1, k\neq i}^{N} (Sinx_i - Sinx_i)$$

Now after some computation and using eq. (1.3), we obtain the first order weighting coefficients of SDQM as

$$A_{ij} = \frac{-P(x_i)Sin^2(x_i)}{(Cosx_i - Cosx_j)Sinx_j P(x_j)} \quad , \ i \neq j \tag{3.18}$$

And

$$A_{ii} = c_i^{(1)}(x_j) + Cotx_i \quad , \tag{3.19}$$

Similarly the weighting coefficient of second order derivative are given by

$$B_{ij} = A_{ij}\left(\frac{2Sinx_i}{(Cosx_i - Cosx_j)} + 2A_{ii} + Cotx_i \ , \ i \neq j\right) \tag{3.20}$$

and

$$B_{ii} = C_i^{(2)}(x_i) + 2Cot(x_i)C_i^{(1)}(x_i) \quad , \quad i = j \tag{3.21}$$

Finally weighting coefficients for the higher order derivatives are given by

$$W_{ij}^{(3)} = 3A_{ij}^{(1)}\left(B_{ii} - \frac{1}{3} + A_{ii}Cotx_i + \frac{Cosx_i}{(Cosx_i - Cosx_j)}\right) + \frac{3Sinx_i B_{ij}^{(1)}}{(Cosx_j - Cosx_i)} \ , i \neq j \tag{3.22}$$

3.4 Cosine Expansion Based Differential Quadrature (CDQM)

Here we consider an even function $g(x)$. Let the Fourier series expansion is used for the approximation of the function $g(x)$ which is of the following form

$$g(x) = d_0 + \sum_{k=1}^{N} d_k Cos(kx) \tag{3.23}$$

There are two sets of base vectors in a $N+1$ linear vector space, which are used to determine the Cosine Expansion Based Differential Quadrature (CDQM)

$$C_k(x) = Cos(kx), k = 0,1,2, \dots, N \tag{3.24}$$

And

$$C_k(x) = \frac{C(x)}{P(x_k)(Cosx - Cosx_k)} \quad , k = 0,1,2, \dots, N \tag{3.25}$$

Where,

$$C(x) = \prod_{k=0}^{N}(Cosx - Cosx_k)$$

$$P(x_i) = \prod_{k=0,k\neq i}^{N}(Cosx_i - Cosx_k)$$

Now after some computation and using equation (1.3), we obtain the first order weighting coefficients of CDQM as

$$A_{ij} = \frac{-P(x_i)Sin(x_i)}{(Cosx_i - Cosx_j)P(x_j)} \quad , \; i \neq j \tag{3.26}$$

and

$$\sum_{j=1}^{N} A_{ij} = 0 \qquad or \qquad A_{ii} = -\sum_{j=1, j\neq i}^{N} A_{ij} \quad , i = j \tag{3.27}$$

Similarly the weighting coefficient of second order derivative are given by

$$B_{ij} = A_{ij}\left(\frac{2Sinx_i}{(Cosx_i - Cosx_j)} + 2A_{ii} + Cotx_i \; , \; i \neq j\right) \tag{3.28}$$

and

$$\sum_{j=1}^{N} B_{ij} = 0 \qquad or \qquad B_{ii} = -\sum_{j=1, j\neq i}^{N} B_{ij} \quad , i = j \tag{3.29}$$

Finally weighting coefficients for the higher order derivatives are given by

$$W_{ij}^{(3)} = 3A_{ij}^{(1)}\left(B_{ii}^{(2)} - \frac{1}{3} + A_{ij}^{(1)}Cotx_i + \frac{Cosx_i}{(Cosx_i - Cosx_j)}\right) + \frac{3Sinx_i B_{ij}^{(2)}}{(Cosx_j - Cosx_i)} \; , i \neq j \tag{3.30}$$

3.5 B-Spline Based Differential Quadrature (BDQM)

In spline base differential quadrature method, instead of using the function values on all grid points to approximate the derivatives as in PDQ, we employ only a small portion of nearby grid points to approximate the derivatives [26, 27]. In this case a uniform partition $a = x_1 < x_2 < \cdots < x_n = b$, of the problem domain $[a, b]$ is considered. Let Q_k, $k = 0,1,2,...N+1$ be a B-spline over the same domain. Forming a basis for the functions defined over $[a, b]$ leads B

-splines to be used as test functions to determine the weighting coefficients w_{ij}^{m} . The use of B-spline functions as test functions in (1.3) leads to the following system of linear equations which can be solved in order to obtain the values of the weighting coefficients:

$$\left.\frac{\partial^m Q_k}{\partial x^m}\right|_{x_i} = \sum_{j=1}^{N} w^{(m)}{}_{ij} Q_k(x_j)\ ,\ \ for\ i = 0,1,2,3,...,N;\ k = 0,1,2,.....,N+1. \qquad \textbf{3.31}$$

Once the weighting coefficients are determine, one can easily use the functional values to compute the derivatives.

3.6 Quintic B-Spline Differential Quadrature Method (QBDQM)

Let $Q_i\ (x)$ be the quintic B-splines with knots at the point x_i where the uniformly distributed grid points are chosen as $a = x_0 < x_1 < \cdots < x_N = b$ on the ordinary real axis with $h = x_i - x_{i-1}, i = 1, \cdots, N$. The quintic B-spline $Q_i\ (x)$ at the knots is given by

$$Q_i(x) = \frac{1}{h^5}\begin{cases} (x - x_{i-3})^5 & ,x \in [x_{i-3}\ , x_{i-2}) \\ (x - x_{i-3})^5 - 6\ (x - x_{i-2})^5 & ,x \in [x_{i-2}, x_{i-1}) \\ (x - x_{i-3})^5 - 6(x - \ x_{i-2})^5 + 15(x - x_{i-1})^5 & ,x \in [x_{i-1}, x_i) \\ (x_{i+3} - x)^5 - \ 6(x_{i+2} - x)^5 + 15\ (x_{i+1} - x)^5 & ,x \in [x_i, x_{i+1}) \\ (x_{i+3} - x)^5 - 6\ (x_{i+2} - x)^5 & ,x \in [x_{i+1}, x_{i+2}) \\ (x_{i+3} - x)^5 & ,x \in [x_{i+2}, x_{i+3}) \\ 0 & otherwise \end{cases}$$

The quintic B-spline $\{Q_{-2}, Q_{-1}, Q_0\ , Q_1, \dots, Q_{N-1}, Q_N, Q_{N+1}, Q_{N+1}\}$ for a basis for the function defined over the domain [a, b] [25, 26, 27, 28, 29]. Each quintic B-spline covers six elements so that each element is covered by six quintic B-splines. The values of $Q_i(x)$ and its derivative are shown in the table 3.1. [25, 26, 27, 28, 29].

Table 3.1. Coefficients of Quintic B-spline and derivatives at x_i

x	x_{i-3}	x_{i-2}	x_{i-1}	x_i	x_{i+1}	x_{i+2}	x_{i+3}
$Q_i(x)$	0	1	26	66	26	1	0
$Q_i'(x)$	0	$\frac{5}{h}$	$\frac{50}{h}$	0	$\frac{-50}{h}$	$\frac{-5}{h}$	0
$Q_i''(x)$	0	$\frac{20}{h^2}$	$\frac{40}{h^2}$	$\frac{-120}{h^2}$	$\frac{40}{h^2}$	$\frac{20}{h^2}$	0
$Q_i'''(x)$	0	$\frac{20}{h^3}$	$\frac{-120}{h^3}$	0	$\frac{120}{h^3}$	$\frac{60}{h^3}$	0
$Q_i''''(x)$	0	$\frac{120}{h^4}$	$\frac{-480}{h^3}$	$\frac{720}{h^4}$	$\frac{-480}{h^4}$	$\frac{120}{h^4}$	0

Using the B-spline as test function in the fundamental DQM equation (1.3) leads to the equation

$$\frac{\partial^n Q_m(x_i)}{\partial x^n} = \sum_{j=m-2}^{m+2} A_{ij}^{(n)}\, Q_m(x_{ji}) \;, i = 0,1,\dots,N, m = -2,-1,\dots,N+1,N+2 \qquad 3.32$$

An arbitrary choice of i leads to an algebraic equation system

$$\begin{pmatrix} Q_{-2,-4} & Q_{-2,-3} & Q_{-2,-2} & Q_{-2,-1} & Q_{-2,-0} & & & & \\ & Q_{-1,-3} & Q_{-1,-2} & Q_{-1,-1} & Q_{-1,0} & Q_{-1,1} & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & & Q_{N+1,N-1} & Q_{N+1,N} & Q_{N+1,N+1} & Q_{N+1,N+2} & Q_{N+1,N+3} & \\ & & & & Q_{N+1,N} & Q_{N+2,N+1} & Q_{N+2,N+2} & Q_{N+2,N+3} & Q_{N+2,N+4} \end{pmatrix} \begin{pmatrix} A_{i,-4}^{(n)} \\ A_{i,-3}^{(n)} \\ . \\ . \\ . \\ A_{i,N+3}^{(n)} \\ A_{i,N+4}^{(n)} \end{pmatrix} =$$

Λ 3.33

Where Q_{ij} represents $Q_i(u_j)$ and $\Lambda = \left[\frac{\partial^n Q_{-2}(x_i)}{\partial x^n}, \frac{\partial^n Q_{-1}(x_i)}{\partial x^n}, \dots, \frac{\partial^n Q_{N+1}(x_i)}{\partial x^n}, \frac{\partial^n Q_{N+2}(x_i)}{\partial x^n}\right]^T$.

The system (3.33) comprise of (N+5) equations and (N+9) unknowns. In order to be able to solve eq. (3.33), four more additional equations are required. We add the following equations

$$\frac{\partial^{n+1} Q_{-2}(x_i)}{\partial x^{n+1}} = \sum_{j=-4}^{0} A_{ij}^{(n)}\, Q'_{-2}(x_j)\,, \frac{\partial^{n+1} Q_{-1}(x_i)}{\partial x^{n+1}} = \sum_{j=-3}^{1} A_{ij}^{(n)}\, Q'_{-1}(x_j)\,,$$

$$\frac{\partial^{n+1} Q_{N+1}(x_i)}{\partial x^{n+1}} = \sum_{j=N-1}^{N+3} A_{ij}^{(n)}\, Q'_{N+1}(x_j)\,, \frac{\partial^{n+1} Q_{N+2}(x_i)}{\partial x^{n+1}} = \sum_{j=N}^{N+4} A_{ij}^{(n)}\, Q'_{N+2}(x_j)$$

to the system (3.33) and using the values of quintic B-spline at the grid points and eliminating $A_{ij,-4}^{(n)}, A_{ij,-3}^{(n)}$, $A_{ij,N+3}^{(n)}$ and $A_{ij,N+4}^{(n)}$ from the system, we obtain an algebraic equation system having penta-diagonal matrix of the form

$$\mathrm{P}A = \Omega \tag{3.34}$$

Where

$$P = \begin{pmatrix} 37 & 82 & 21 & & & & & & \\ 8 & 33 & 18 & 1 & & & & & \\ 1 & 26 & 66 & 26 & 1 & & & & \\ & 1 & 26 & 66 & 226 & 1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 1 & 26 & 66 & 26 & 1 & \\ & & & & 1 & 26 & 66 & 26 & 1 \\ & & & & & 1 & 18 & 33 & 8 \\ & & & & & & 21 & 82 & 37 \end{pmatrix} \text{ And } A = \begin{pmatrix} A_{i,-2}^{(n)} \\ A_{i,-1}^{(n)} \\ \vdots \\ A_{i,j-2}^{(n)} \\ A_{i,j-1}^{(n)} \\ A_{i,j}^{(n)} \\ A_{i,j+1}^{(n)} \\ A_{i,j+2}^{(n)} \\ \vdots \\ A_{i,N+1}^{(n)} \\ A_{i,N+2}^{(n)} \end{pmatrix}$$

The entries of the load vector Ω are given as:

$$\Omega_{-2} = \frac{1}{30}\left(-5Q_{-2}^{(n)}(x_i) + hQ_{-2}^{(n+1)}(x_i) + 40Q_{-1}^{(n)}(x_i) + 8hQ_{-1}^{(n+1)}(x_i)\right)$$

$$\Omega_{-1} = \frac{1}{10}\left(5Q_{-1}^{(n)}(x_i) - hQ_{-1}^{(n+1)}(x_i)\right)$$

$$\Omega_{i-2} = Q_{i-2}^{(n)}, \Omega_{i-1} = Q_{i-1}^{(n)}, \Omega_i = Q_i^{(n)}, \Omega_{i+1} = Q_{i+1}^{(n)}, \ \Omega_{i+2} = Q_{i+2}^{(n)},$$

$$\Omega_{N+1} = \frac{1}{10}\left(5Q_{N+1}^{(n)}(x_i) - hQ_{N+1}^{(n+1)}(x_i)\right),$$

$$\Omega_{N+2} = \frac{-1}{30}\left(5Q_{N+2}^{(n)}(x_i) + hQ_{N+2}^{(n+1)}(x_i) + 40Q_{N+1}^{(n)}(x_i) + 8hQ_{N+1}^{(n+1)}(x_i)\right) \tag{3.35}$$

The system of equations (3.34) can be solved by using Thomas algorithm at each grid point $x_i, i = 0,1,2, \dots, N$ and we can get all the weight coefficients $A_{i,j}^{(n)}$, for all $i, j = 0,1, \dots N, n = 1, \dots, N-1$.

4. Numerical Experiments

In this section numerical solutions are studied for Schrödinger equations (2.35). In order to understand the applicability of the DQM two test problems, namely single soliton and soliton interactions are solved separately using the quintic B-spline based DQM and the result obtain are compared with the analytical solutions and with the earlier numerical solutions [34, 35].

The Schrödinger equations for the test problems can be written as follows:

$$i\psi_t = -\psi_{xx} - q\psi|\psi|^2 = 0\,, (x,t) \in (-\infty,\infty) \times (0,T)\,. \tag{4.1}$$

Where $i = \sqrt{-1}$, $\psi(x,t)$ is a complex valued function, which represents weakly nonlinear, strongly dispersive and almost monochromatic [34], x is the spatial coordinate, t is time, q is a real parameter and ψ_t , ψ_{xx} represents derivative with respect to t and x respectively. In order to solve eq. (4.1) numerically artificial boundary conditions are introduce $\psi(a,0) = \psi(b,0) = 0$ to model the physical conditions.

Assuming,

$$\psi(x,t) = f(x,t) + ig(x,t) \tag{4.2}$$

Where, $f(x,t)$ and $g(x,t)$ are real functions.

We have

$$\psi_t = f_t + ig_t$$

$$\psi_{xx} = f_{xx} + ig_{xx} \tag{4.3}$$

Substituting system (4.3) in to eq. (4.1) the following system of equations are obtained,

$$g_t = f_{xx} + q(f^2 + g^2)f$$

$$f_t = -g_{xx} - q(f^2 + g^2)g \tag{4.4}$$

And the corresponding boundary conditions are:

$$g(a,t) = f\,(a,t) = 0$$

$$g(b,t) = f(b,t) = 0. \quad 4.5$$

Use of DQM approximations described in section (3.6) for spatial discretization of (4.4) leads to the following ODE's system.

$$\left.\frac{\partial g}{\partial t}\right|_{x=x_i} = \sum_{j=0}^{N} A_{ij}^{(2)} f_j + q(f_i^2 + g_i^2) f_i$$

$$\left.\frac{\partial f}{\partial t}\right|_{x=x_i} = -\sum_{j=0}^{N} A_{ij}^{(2)} g_j - q(f_i^2 + g_i^2) g_i \quad (4.6)$$

Where the weighting coefficients are given in section (3.6). The above system of equations (4.6) are solved using RK4 method.

To get a reliable solution it is important to consider discrete conservation laws for the computation of smooth solitons of (4.1). Here, we have considered two basic conserved quantities as follows:

$$C_1 = \int_a^b |\psi|^2 dx \approx \sum_{j=0}^{N} |\psi_j^n|^2 \quad 4.7$$

$$C_2 = \int_a^b \left(|\frac{\partial \psi}{\partial x}|^2 - \frac{1}{2} q |\psi|^4 \right) dx \quad 4.8$$

Where $\psi(x,t)$ is the analytical solution and ψ_j^n is the numerical solution at n^{th} time step at j[th] node.

Further to determine the error we have used L_∞ defined as follow

$$L_\infty = \max_j |\psi_j - \psi_j^n| \quad 4.9$$

4.1 Results and Discussion

Single Solitary Solution:

The analytical solution of (4.1) is of the form [34]

$$\psi(x,t) = \beta \sqrt{\frac{2}{q}} \exp i \left(\frac{cx}{2} - \frac{(c^2 - \beta^2)t}{4} \right) \times Sech(\beta(x - ct)) \quad 4.10$$

Where *c* represents the speed of the single soliton and its magnitude depends on α.

Putting $t = 0$ in the solution expression (4.10) we get the initial expression as $\psi(x, 0)$.

The system of first order ODE's (4.6) are solve under the boundary conditions (4.5) and the initial condition $\psi(x, 0)$ for suitable values of parameters in order to compare our present results with the analytical solutions and the earlier results [34, 35]. For $q = 2, c = 4, \beta = 1$, the soliton,

$$|\psi| = Sech(x - 4t) \qquad 4.11$$

propagates to the right with unchanged profiles at a constant speed of $c = 4$. Fig.1 depicts the propagation of the single soliton at different times. Using the above parameters with $h = 0.1$, and $\Delta t = 0.001$ numerical results obtained by our method are tabulated in the table 4.1.

Table 4.1. Conserved Quantities and Errors with $h = 0.1, \Delta t = 0.001, N = 400$

t	C_1	C_2	Max. error
0	2.000000	-0.666711	00000
0.5	2.000000	-0.666657	1.84234×10^{-6}
1	2.000000	-0.66667	2.4968×10^{-6}
1.5	2.000000	-0.66667	3.12936×10^{-6}
2	2.000000	-0.666657	4.01783×10^{-6}

Table 4.2 Errors with $h = 0.1, \Delta t = 0.001, N = 400$

t	Max. error
0	00000
1	1.162331×10^{-5}
2	2.301020×10^{-5}

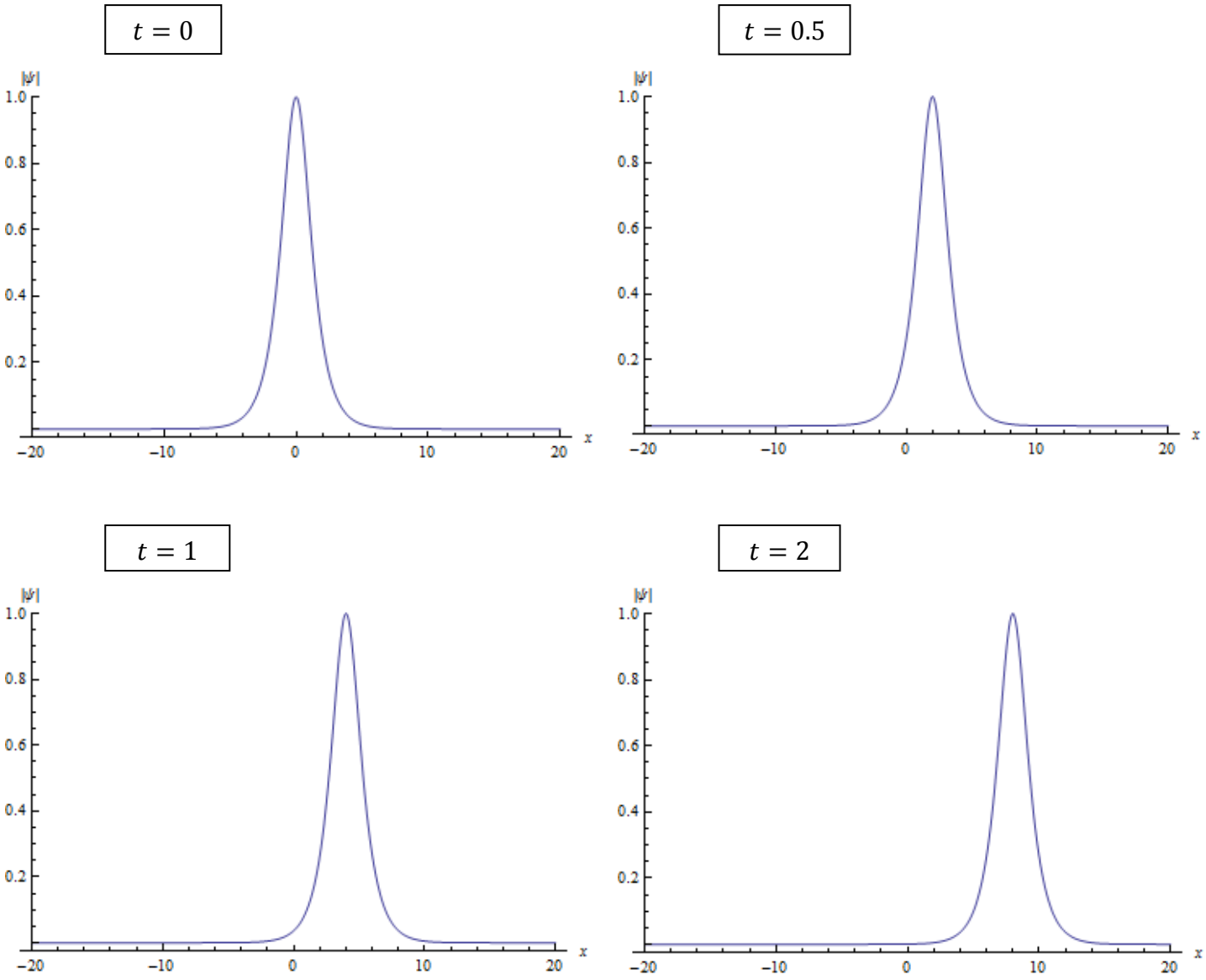

Fig.1 Single Solitary at different times , $N = 400$

In order to know the efficiency of our present QBDQM we used the Cosine based differential method with same parameters and the numerical results are tabulated in the table 4.2

We have compared the errors with some the earlier works [34, 35] and presented in Table 4.3.

Table 4.3 Comparison of single soliton at time $t = 1$ with some earlier results

Method	h	Δt	L_∞
Quintic B-spline(present)	0.1	0.001	2.4968×10^{-6}
CDQM(present)	0.1	0.001	1.162331×10^{-5}
B-spline Galerkin [34]	0.05	0.005	0.0003
Hopscotch [34]	0.08	0.002	0.005
Split-step Fourier [34]	0.3125	0.020	0.005
Pseudospectral [34]	0.3125	0.00026	0.005

Interaction of two Solitons

For the interaction of two solitons the initial condition is given as [34]

$$\psi(x,0) = \psi_1(x,0) + \psi_2(x,0) \tag{4.12}$$

Where

$$\psi_j(x,0) = \beta_j\sqrt{\frac{2}{q}}exp\left\{\frac{1}{2}\,S_j(x-x_j)\right\} \times Sech\,\beta_j(x-x_j)$$

The system of first order ODE's (4.6) are solve under the boundary conditions (4.5) and the initial condition (4.12) for suitable values of parameters. We have considered the parameters $q = 2, \beta_1 = 1, \beta_2 = 1, S_1 = 4, S_2 = -4, x_1 = -10, x_2 = 10, h = , \Delta t = 0.01$. The initial condition given by equation (4.12) represents two solitons of equal magnitudes and they are separated by a distant of 20 units, first one is placed at $x_1 = -10$ and second one is placed at $x_2 = 10$, both with equal and opposite velocities. The interaction of two soliton at different times are shown in the figure 2 , we observed that two waves travelling in opposite direction after the collision separate but conserve their initial shapes.

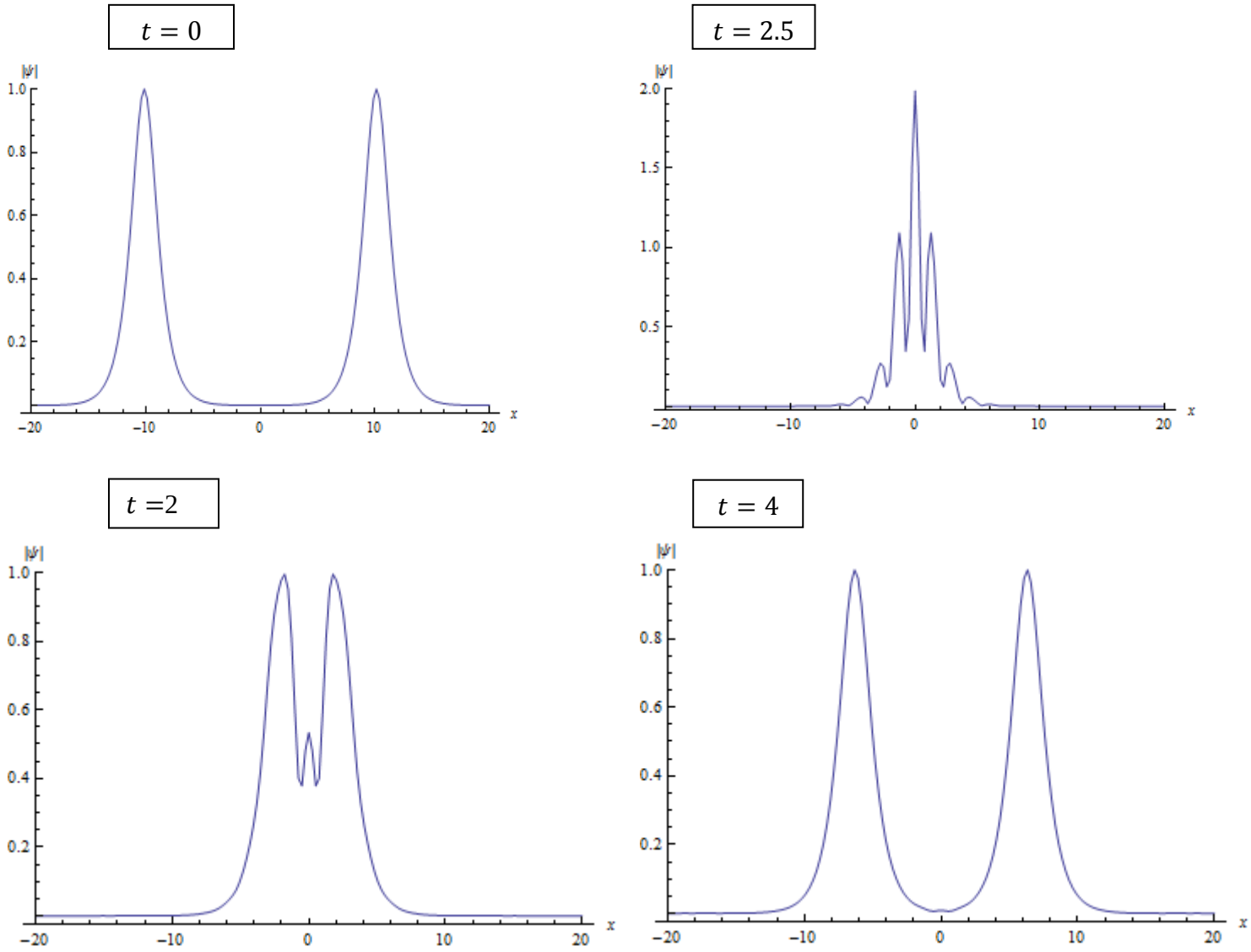

Fig.2 Interaction of two solitons (N=200)

Numerical results obtained by our method and Cosine based differential method are tabulated in the table 4.4 and table 4.5 respectively.

Table 4.4 Conserved Quantities and variants with $q = 2, \beta_1 = 1, \beta_2 = 1, S_1 = 4, S_2 = -4, x_1 = -10, x_2 = 10, h = , \Delta t = 0.01$ $h = 0.25$ $, \Delta t = 0.01, N = 200$

t	C_1	C_2	$\frac{C_1 - C_1^0}{C_1^0}$	$\frac{C_2 - C_2^0}{C_2^0}$
0	3.99991	-1.33332	----	----
1	3.99992	-1.33329	0.0000025	-0.000022500
2	3.99946	-1.33335	-0.0001125025	0.0000225002
2.5	3.99993	-1.33333	0.0000050001	0.0000075001
4	3.99994	-1.33323	0.0000075002	0.0000675007

Table 4.5. Conserved Quantities and variants with $q = 2, \beta_1 = 1, \beta_2 = 1, S_1 = 4, S_2 = -4, x_1 = -10, x_2 = 10, h = , \Delta t = 0.01$ $h = 0.25$ $, \Delta t = 0.01, N = 200$

t	C_1	C_2	$\frac{C_1 - C_1^0}{C_1^0}$	$\frac{C_2 - C_2^0}{C_2^0}$
0	3.99999	-1.33340	----	----
1	3.99992	-1.33329	-0.0000175	-0.000082495
2	3.99996	-1.33337	-0.0000075	-0.000022498

We have also done a comparison of the conserved quantities and relative changes of the conserved quantities at $t = 1$ with some of the earlier works [34, 35] and shown in the table 4.6.

Table 4.6. Comparison of two soliton simulations at time $t = 2.5$ *with some earlier results*

Method	h	$\boldsymbol{\Delta t}$	$\boldsymbol{\frac{C_1 - C_1^0}{C_1^0}}$	$\boldsymbol{\frac{C_2 - C_2^0}{C_2^0}}$
Quintic B-spline(present)	0.25	0.01	0.0000050001	0.0000075001
CDQM(present)	0.25		-0.00000740	-0.000022498
B-spline Galerkin [34]	0.10	0.01	-0.000003	0.00330
Hopscotch [34]	0.05	0.001	0.000030	0.00063
Split-step Fourier [34]	0.625	0.005	0.000710	0.03595
Pseudospectral [34]	0.625	0.0071	0.00073	0.03247

5. Solution of Coupled Nonlinear Schrodingr Equation

In this chapter we study the nemerical results of the Coupled Nonlinear Schrödinger Equation (CNLSE) of the form [30]

$$i\frac{\partial\psi_1}{\partial t}+\frac{1}{2}\frac{\partial^2\psi_1}{\partial x^2}+(|\psi_1|^2+\epsilon|\psi_2|^2)\psi_1=0\,,\qquad x\in(-\infty,\infty)\,, \tag{5.1}$$

$$i\frac{\partial\psi_2}{\partial t}+\frac{1}{2}\frac{\partial^2\psi_2}{\partial x^2}+(\epsilon|\psi_1|^2+|\psi_2|^2)\psi_2=0\,,\qquad x\in(-\infty,\infty)\,, \tag{5.2}$$

with boundary conditions:

$$i\frac{\partial\psi_1(x,t)}{\partial x}=i\frac{\partial\psi_2(x,t)}{\partial x}=0\ \text{ as } |x|\to\infty \tag{5.3}$$

Where ψ_1 and ψ_2 are the wave amplitudes in two polarizations and e represents the the cross-phasde modulation coefficient. Where $i=\sqrt{-1}$, $\psi_1(x,t)$ and $\psi_1(x,t)$ are complex valued function, *x* is the spatial coordinate, *t* is time. In order to solve eq. (5.1 and 5.2) numerically we assume

$$\psi_1(x,t)=f_1(x,t)+ig_1(x,t) \tag{5.4}$$

$$\psi_2(x,t)=f_2(x,t)+ig_2(x,t). \tag{5.5}$$

Where, $f_1(x,t), g_1(x,t), f_2(x,t)\ and\ g_2(x,t)$ are real functions.

We have

$$\frac{\partial\psi_1}{\partial t}=\frac{\partial f_1}{\partial t}+i\frac{\partial g_1}{\partial t}$$

$$\frac{\partial\psi_2}{\partial t}=\frac{\partial f_2}{\partial t}+i\frac{\partial g_2}{\partial t}$$

$$\frac{\partial^2\psi_1}{\partial x^2}=\frac{\partial^2 f_1}{\partial x^2}+i\frac{\partial^2 g_1}{\partial x^2}$$

$$\frac{\partial^2\psi_2}{\partial x^2}=\frac{\partial^2 f_2}{\partial x^2}+i\frac{\partial^2 g_2}{\partial x^2} \tag{5.6}$$

Substituting system (5.6) in the system of eq. (5.1, 5.2) the following system of equations are obtained

$$i\left(\frac{\partial f_1}{\partial t}+i\frac{\partial g_1}{\partial t}\right)+\frac{1}{2}\left(\frac{\partial^2 f_1}{\partial x^2}+i\frac{\partial^2 g_1}{\partial x^2}\right)+(|f_1+ig_1|^2+\epsilon|f_2+ig_2|^2)(f_1+ig_1)=0 \quad 5.7$$

$$i\left(\frac{\partial f_2}{\partial t}+i\frac{\partial g_2}{\partial t}\right)+\frac{1}{2}\left(\frac{\partial^2 f_2}{\partial x^2}+i\frac{\partial^2 g_2}{\partial x^2}\right)+(\epsilon|f_1+ig_1|^2+|f_2+ig_2|^2)(f_2+ig_2)=0 \quad 5.8$$

And the corresponding boundary conditions are:

$$i\left(\frac{\partial f_1(x,t)}{\partial x}+\frac{\partial g_1(x,t)}{\partial x}\right)=i\left(\frac{\partial f_2(x,t)}{\partial x}+\frac{\partial g_2(x,t)}{\partial x}\right)=0 \quad 5.9$$

Use of DQM approximations described in section (3.6) for spatial discretization of the system (5.7, 5.8) leads to the following ODE's system.

$$\frac{\partial g_1}{\partial t}=\frac{1}{2}\left(\sum_{j=0}^{N}A_{ij}^{(2)}f_{1j}\right)+(|\psi_1|^2+\epsilon|\psi_2|^2)f_1$$

$$\frac{\partial f_1}{\partial t}=-\frac{1}{2}\left(\sum_{j=0}^{N}A_{ij}^{(2)}g_{1j}\right)-(|\psi_1|^2+\epsilon|\psi_2|^2)g_1$$

$$\frac{\partial g_2}{\partial t}=\frac{1}{2}\left(\sum_{j=0}^{N}A_{ij}^{(2)}f_{2j}\right)+(\epsilon|\psi_1|^2+|\psi_2|^2)f_2$$

$$\frac{\partial f_2}{\partial t}=-\frac{1}{2}\left(\sum_{j=0}^{N}A_{ij}^{(2)}g_{2j}\right)-(\epsilon|\psi_1|^2+|\psi_2|^2)g_2 \quad 5.10$$

Where the weighting coefficients are given in section (3.6). The above system of ODE`s (5.10) are solved using RK4 method.

5.1 Results and Discussion

Single Solitary Solution:

The analytical solution of (5.1, 5.2) are of the form [30]

$$\psi_1(x,t)=\sqrt{\frac{2\alpha}{1+\upsilon}}Sech\sqrt{2\alpha}(x-ct)\exp i\left\{cx-\left[\frac{c^2}{2}-\alpha\right]t\right\}\ ,$$

$$\psi_2(x,t)=\sqrt{\frac{2\alpha}{1+\upsilon}}Sech\sqrt{2\alpha}(x-ct)\exp i\left\{cx-\left[\frac{c^2}{2}-\alpha\right]t\right\}\ , \quad 5.11$$

Putting $t=0$ in the solution expression (5.11) we get the initial expression as $\psi_1(x,t)$ and $\psi_2(x,t)$.

The system of first order ODE's (5.10) are solve under the boundary conditions (5.9) and the initial condition $\psi_1(x,0)$ and $\psi_2(x,0)$ for suitable values of parameters. For $\upsilon=1, c=1,$

$\alpha = 1$ with $h = 0.1$, and $\Delta t = 0.01$ numerical results obtained by our method for ψ_1 and ψ_2 are tabulated in the table 5.1. and 5.2 respectively. Fig 3 depicts the evolution of single soliton moving to the right with velocity $c = 1$.

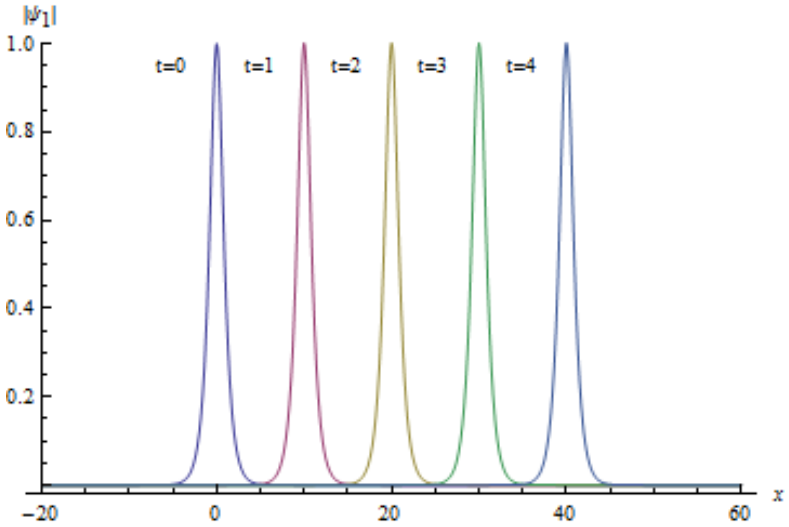

Fig.3. Single Solitary at different times , $N = 800$

Table 5.1. Conserved Quantities and Errors with $h = 0.1 , \Delta t = 0.01, N = 800$

t	c_1	c_2	L_∞
0	1.41421	0.470532	----
1	1.41421	0.470670	3.493400×10^{-5}
2	1.41421	0.470672	5.906480×10^{-5}
3	1.41421	0.470656	7.747943×10^{-5}
4	1.41421	0.470660	8.133650×10^{-5}

Table 5.2. Conserved Quantities and Errors with $h = 0.1 , \Delta t = 0.01, N = 800$

t	c_1	c_2	L_∞
0	1.41421	0.470532	----
1	1.41421	0.470670	3.46105×10^{-5}
2	1.41421	0.470672	5.88181×10^{-5}
3	1.41421	0.470656	7.44700×10^{-5}
4	1.41421	0.470660	8.08233×10^{-5}

We have also compared our results with some of the earlier works [30, 31, 32, 33] which are tabulated in the table 5.3

Table 5.3 Comparison of single soliton at time $t = 1$ *with some earlier results*

Method	h	$\boldsymbol{\Delta t}$	$\boldsymbol{L_\infty}$
Quintic B-spline(present)	0.100	0.01	3.493400×10^{-5}
Galerkin [30]	0.100	0.01	0.01722
Meshless Local Petrov–Galerkin [31]	0.025	0.001	1.2375×10^{-4}
Direct-discontinuous Galerkin method [32]	0.500	0.01	6.2914×10^{-4}

6. Conclusion

From our results it is clear that our present method (QBDQM) out performs some of the conventional numrical methods like Hopscotch , Psuedo-spectral , Galerkin [30], Meshless Local Petrov–Galerkin [31], as well as other global DQMs like PDQM and CDQM. Global DQMs are insuficient when the number of grid points are large and small number grid points greately limit the applications og local DQMs. For example a solitary wave sweeps all parts of space. The grid points should be uniformly distributed to correctly capture wave profiles at different time steps but fewer grid points deterioates wave profile as time increases. The localised DQMs like our method (QBDQM) overcomes these limitations. In table 4.3, 4.6, 5.3 we have listed the values of error corresponding to some of the earlier methods as well as our method and it is clear form the tabulated values that error corresponding to our method are minimum.

REFERENCE

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