CONSERVATIVE SCHEMES FOR THE THREE COUPLED NONLINEAR SCHRÖDINGER EQUATION

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ABSTRACT

Conservative schemes for the three coupled nonlinear Schrödinger equation

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The N-coupled nonlinear Schrödinger (N–CNLS) equation is one of the highly used mathematical models in many scientific areas including physics, optics, quantum mechanics and fluid dynamics. In recent years, although there are many numerical studies on the nonlinear Schrödinger (NLS) equation and coupled NLS (2–CNLS) equation, numerical studies on three coupled NLS (3–CNLS) equation are rare. This system of equations has some physical (or geometric) properties such as mass (or charge) and energy conservations. Standard numerical schemes do not preserve these properties and usually these properties are destroyed in the numerical solution. Recently, constructing conservation methods that preserves this type of physical properties has an increasing interest among the researchers. The purpose of this thesis is to develop some conservative methods that preserve one or more physical properties of the 3–CNLS equation. Two conserved quantities, namely energy and mass conservations of 3–CNLS equation are obtained. Then, three numerical schemes are constructed that preserve the discrete versions of these conserved quantities under some suitable boundary conditions such as periodic or homogenous boundary conditions. First, an energy preserving algorithm is proposed by using a method known as Average Vector Field (AVF) method. Then, a two–step (or three level) scheme is proposed that preserves the mass of the equation. Finally, a one–step scheme (or two level scheme) is proposed for the numerical solution of the equation that preserves both the energy and the mass of the equation. Linear stability, accuracy and convergence of these methods are discussed. Dispersion relations of the energy preserving scheme and the mass conserving schemes are analyzed. Many numerical experiments are performed to verify the efficiency and invariant conservation property of the schemes. Numerical results show that the new methods constructed here have excellent performance in simulating the periodic, single and colliding soliton solutions of the equation in long time.

Keywords: Three coupled nonlinear Schrödinger equation, geometric integration, dispersion relation, solitary wave, periodic wave

ÖZ

Üçlü lineer olmayan Schrödinger denklemi için yapı koruyan sayısal yöntemler

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Birleşik N denklemli lineer olmayan Schrödinger (N–CNLS) denklemi fizik, optik, kuantum mekaniği ve akışkanlar dinamiği gibi birçok alanda sıklıkla kullanılan önemli matematiksel modellerden biridir. Son yıllarda lineer olmayan Schrödinger (NLS) denklemi ve ikili lineer olmayan Schrödinger (2-CNLS) denklemi için yapılmış çok sayıda çalışma varken, üçlü lineer olmayan Schrödinger (3-CNLS) denklem sistemi için yapılan sayısal çalışma sayısı oldukça azdır. Bu denklem sistemlerinin kütle korunumu ve enerji korunumu gibi bazı fiziksel (ya da geometrik) korunum özellikleri vardir. Standard sayısal yöntemler bu tür korunumları korumamakta ve korunum sayısal çözümde bozulmaktadır. Son yıllarda bu tip özellikleri koruyan sayısal yöntemler geliştirme çalışmalarına ilgi araştırmacılar arasında hızla artmaktadır. Bu tezin amacı, üçlü lineer olmayan Schrödinger (3-CNLS) denkleminin bir veya birden fazla fiziksel (ya da geometrik) özelliğini koruyan sayısal yöntemler geliştirmektir. 3-CNLS denkleminin enerji ve kütle olmak üzere iki korunum özelliği elde edilmiştir. Daha sonra, periyodik ve homojen sınır şartları gibi uygun sınır şartları altında, bu korunumların ayrık hallerini koruyan üç tane sayısal yöntem geliştirilmiştir. İlk olarak, Ortalama Vektör Alanı (AVF) olarak bilinen bir yöntem kullanılarak, enerji koruyan sayısal yöntem tasarlanmıştır. Daha sonra denklemin kütlesini koruyan iki adımlı (ya da üç basamaklı) bir sayısal yöntem tasarlanmıştır. Son olarak, denklemin hem kütle hem de enerjisini koruyan bir adımlı (ya da iki basamaklı) sayısal yöntem tasarlanmıştır. Tasarlanan sayısal yöntemlerin doğrusal kararlılık, doğruluk ve yakınsaklık analizleri yapılmıştır. Enerji ve kütle koruyan sayısal yöntemlerin dağılım özellikleri incelenmiştir. Sayısal yöntemlerin etkinliğini ve yapı koruma özelliklerini doğrulamak için bir çok sayısal uygulamalar yapılmıştır. Sayısal sonuçlar uzun zaman aralığında her üç sayısal yöntemin de denklemin periyodik, bir soliton ve çarpışan soliton çözümlerinin de çok iyi sonuçlar verdiğini göstermektedir.

Anahtar Kelimeler: Üçlü lineer olmayan Schrödinger denklemi, yapı koruyan sayısal yöntem, dağılım denklemi, soliter dalga, periyodik dalga

To My Parents

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CHAPTER 1

PRELIMINARIES

In this chapter, we shall introduce the concept of the geometric integration by using the equation of simple harmonic oscillator. Then, we will introduce the single nonlinear Schrödinger (NLS) equation and the 2–coupled nonlinear Schrödinger (2–CNLS) equation. We will summarize the recent numerical methods that are proposed for the numerical solutions of NLS and 2–CNLS equations.

1.1 Historical Bibliography

Efficient and accurate numerical methods for approximate solutions of initial value problems (IVP) and/or boundary value problems (BVP) for the differential equations appearing in physics, engineering and in the other fields of sciences have been a goal of scientists for decades. One can argue that there are four traditional numerical ”techniques” for the numerical solution of ordinary differential equations (ODEs) and partial differential equations (PDEs); namely, finite difference, finite element, spectral and meshfree methods. Each technique started to appear in mathematics literature in successive decades, namely finite difference methods in the 1950s, the finite element methods in the 1960s, spectral methods in the 1970s and meshfree methods in the 1980s.

The finite difference methods are still one of the most important and useful mathematical tool for engineers and scientists. It remains as a fundamental technique in many software programmes.

Many practical problems in science and engineering are PDE and involve conserved quantities such as conservation of mass and/or conservation of energy and lead to PDE of this type of involvement class. A PDE, in principal, can be solved by using the inverse scattering transform [1, 2]. But, this solution is not the general solution; it is a special case which is known as soliton solutions. In fact, we know much about the mathematical structure of these equations and their solutions, such as conserved quantity and symmetry. Therefore, in order to understand the dynamics of the complete soliton of the model, we have to develop some numerical algorithms. But in numerical solutions of these problems, the mathematical structures such as conserved quantity and symmetry, are not generally preserved. Therefore, it is natural to develop an algorithm that preserves these properties. Preservation of such structures of differential equations by numerical integration methods has been the subject of many researches [3]. The theory of structure preserving algorithms is developed in different areas of science such as celestial mechanics [4] and molecular dynamics [5]. Numerical experiments have shown that the structure preserving schemes give better results than the non-preserving schemes. In addition, structure preserving schemes are efficient in long time simulation and do not show blow-up [6]. Conservation of energy has a priority and has a far reaching importance within the topic of the conservation properties. Several works have been done about this structures for the differential equations. In [7], two energy conserving schemes are presented for Sine- Gordon equation. In [8, 9] and [10], some conservative methods have been developed for Rosenou-KdV equation, regularized long wave equation and Schrödinger Bousinessq equation, respectively.

A numerical method designed to preserve some qualitative structures of the differential equation may also preserve additional properties of the equation. For example, symplectic methods are designed for Hamiltonian differential equations that preserve the symplectic structure of the Hamiltonian system. In addition they have excellent performance on energy preservation (due to the backward error analysis), and can conserve angular momentum and other invariants of the Hamiltonian system [3]. Hamiltonian differential equation is written in the form

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i}, \quad i = 1, 2, \cdots, d \tag{1.1}$$

where the Hamiltonian $H(x(t), p(t)) : \mathbb{R}^{2d} \to \mathbb{R}$ is a real-valued function. The vector $x = (x_1, x_2, \cdots, x_d)$ represents the generalized coordinates of the system i.e. position or angles, $p = (p_1, p_2, \cdots, p_d)$ is the set of generalized momenta in mechanics and d is the degrees of freedom's of the Hamiltonian system. Hamiltonian (or the energy) can be expressed as sum of kinetic energy and the momentum energy. It is a constant of the motion, that is

$$\begin{aligned} \frac{d}{dt}H(x(t), p(t)) &= \sum_{i=1}^{d} \frac{\partial H}{\partial x_i}\dot{x}_i + \sum_{i=1}^{d} \frac{\partial H}{\partial p_i}\dot{p}_i \\ &= \sum_{i=1}^{d} \frac{\partial H}{\partial x_i}\left(\frac{\partial H}{\partial p_i}\right) + \frac{\partial H}{\partial p_i}\left(-\frac{\partial H}{\partial x_i}\right) \\ &= 0 \end{aligned} \tag{1.2}$$

i.e.

$$H(x(t), p(t)) = \text{ const}$$

for all time t. If $H(x, p) = T(x) + U(p)$, then the system (1.1) is said to be **seperable**. A remarkable property of the Hamiltonian system (1.1) is the symplecticity of its true flow [11]. In one-degree of freedom ($d = 1$) symplecticity implies preservation of area. In higher dimension ($d > 1$), it corresponds to preservation of volume under flow map. A numerical one–step method is said to be

symplectic if it preserve the symplectic structure of the Hamiltonian system. An example for the symplectic method is the the implicit midpoint method. A necessary and sufficient condition for a Runge–Kutta method with Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}, \qquad b, c \in \mathbb{R}^d, A \in \mathbb{R}^{d\times d}$$

to be symplectic is that

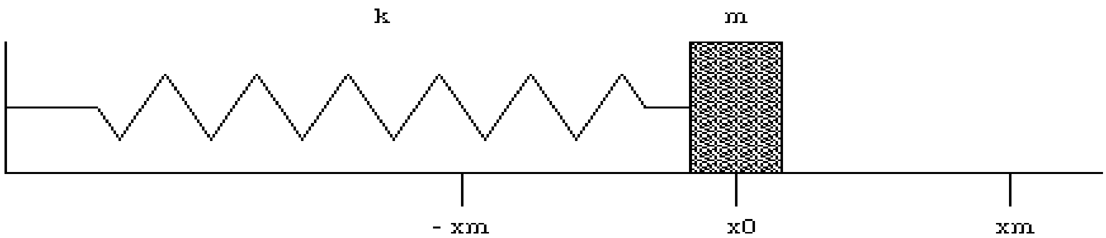
$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$$

for all $i, j = 1, 2, \cdots, d$. (see [11]). In the geometric integration context, it is well known that symplectic Runge–Kutta method preserves all quadratic invariants. In the following example, we will illustrate this fact by applying the conservative implicit midpoint method and non-conservative Euler method to the harmonic oscillator equation as a Hamiltonian system.

A one dimensional simple harmonic oscillator is a second-order ODE

$$m\frac{d^2x}{dt^2} + kx = 0, \tag{1.3}$$

which describes by a mass-spring system with potential energy $\frac{1}{2}kx^2$ and the kinetic energy $\frac{1}{2}kp^2$. Here, m represents the mass of the spring and k is the spring constant. The solution of this equation, $x(t)$, gives the position x of the oscillator at any time t.



The equation (1.3) has a separable Hamiltonian

$$H(x, p) = \frac{1}{2}kx^2 + \frac{p^2}{2m}. \tag{1.4}$$

The associated Hamiltonian differential equations can be written as

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p} = p/m, \\ \dot{p} &= -\frac{\partial H}{\partial x} = -kx. \end{aligned} \tag{1.5}$$

In the first equation $\dot{x}$ represents the velocity of the particle, $v = p/m$. The second equation $\dot{p} = m\dot{v} = ma = F$ gives the force law corresponding to the potential energy $\frac{1}{2}kx^2$ on the spring. Note that for the parameters $m = k = 1$, the Hamiltonian (1.4) is the circle

$$\Gamma(t) \equiv x(t)^2 + p(t)^2 = C^2, \text{ for all } t \tag{1.6}$$

where C is a constant. Applying the forward Euler method to the Hamiltonian system (1.5) with $k = m = 1$ and choosing h as the size, we get,

$$\begin{aligned} x_{n+1} &= x_n + h\ p_n, \\ p_{n+1} &= p_n - h\ x_n \end{aligned} \tag{1.7}$$

and the implicit midpoint rule for the same system yields

$$\begin{aligned} x_{n+1} &= x_n + h\ \left(\frac{p_{n+1} + p_n}{2}\right), \\ p_{n+1} &= p_n - h\ \left(\frac{x_{n+1} + x_n}{2}\right). \end{aligned} \tag{1.8}$$

We see that, in the case of the Euler scheme (1.7), Γ in (1.6) evolves through the solution (1.7), to the new circle given by

$$x_{n+1}^2 + p_{n+1}^2 = (1 + h^2)\left(x_n^2 + p_n^2\right) = (1 + h^2)C^2, \tag{1.9}$$

which can be seen in the Figure 1.1(a). Note that the area enclosed by the discrete solution $(x_n, p_n)^T$ has increased by a factor of $1 + h^2$. Figure 1.1(b) shows the increasing oscillation in time. In the case of the implicit midpoint rule (1.8), it can be shown that Γ is mapped to the same circle

$$x_{n+1}^2 + p_{n+1}^2 = x_n^2 + p_n^2 \tag{1.10}$$

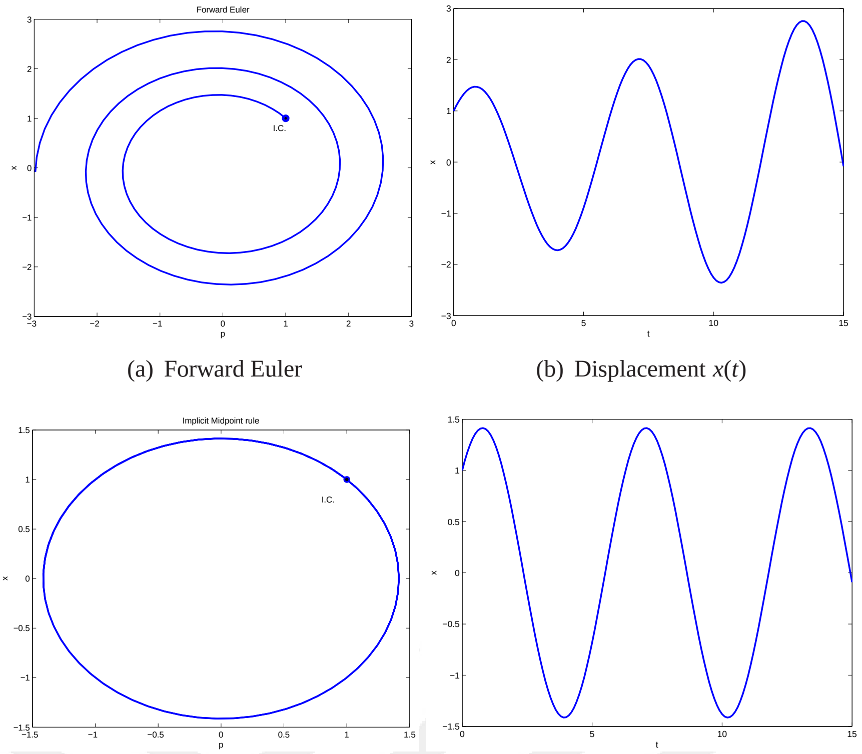
so that

$$x_{n+1}^2 + p_{n+1}^2 = x_n^2 + p_n^2 = \cdots = x_0^2 + p_0^2 = C^2, \tag{1.11}$$

where $x_0^2 + p_0^2 = C^2$ represents the circle at the initial time $t = 0$. This phenomenon can be seen in the Figure 1.1(c). Figure 1.1(d) shows the periodic oscillation of the position x with respect to time t. Notice that after some time the position x reaches the same point. One can conclude that the implicit midpoint rule (1.8) is a conservative scheme for the simple harmonic oscillator (1.3) that conserves the property (1.6).

In numerical analysis, an ODE can be classified as stiff and non stiff equation. For stiff equations implicit Runge–Kutta (RK) methods turned out to be suitable solver. However, for non stiff equations an ideal method is explicit ones. For Hamiltonian systems there exist symplectic methods that preserve a quadratic conservation law on first variations of solutions.

In the last several decades, there has been a great deal of interest for numerical solution of ODE or PDEs while preserving one or more (geometric) properties up to round–off error (see [3, 12] and reference therein). It is well known that all Runge–Kutta (RK) methods preserves linear invariants [13] and symplectic RK methods preserves quadratic invariants of Hamiltonian systems [14]. Symplectic integrators, in general do not exactly conserve the Hamiltonian. The discrete Hamiltonian displays an oscillating behavior. The amplitude of the oscillation is bounded with respect to the time and the Hamiltonian is nearly conserved.



(a) Forward Euler (b) Displacement $x(t)$

(c) Implicit midpoint rule (d) Displacement $x(t)$

Figure 1.1: Simple Harmonic Oscillator. Left: Phase Portraits; Right: Displacement

However, for polynomial Hamiltonian functions of degree greater than two, such conservation properties are lost [15]. Iavernaro et.al [16] introduced a class of s–stage trapezoidal methods that exactly preserves a polynomial Hamiltonian function of separable Hamiltonian system. Recently, an energy preserving B–series method has been proposed in [17]. It is called ”average vector field” (AVF) method and described as a novel class of B-series methods that preserves the energy for all Hamiltonian vector fields [19]. For the differential equation

$$\frac{du}{dt} = f(u), \quad u \in \mathbb{R}^n \tag{1.12}$$

the second order AVF method is given by [17]

$$\frac{u_{n+1} - u_n}{\Delta t} = \int_0^1 f((1-\xi)u_n + \xi u_{n+1})\, d\xi. \tag{1.13}$$

For example, if $f(u) = u$, then the integral turns into

$$\int_0^1 f((1-\xi)u_n + \xi u_{n+1})\, d\xi = \frac{u_{n+1} + u_n}{2},$$

which means that the scheme (1.13) is equivalent to the well known implicit midpoint rule

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{u_{n+1} + u_n}{2}. \tag{1.14}$$

If $f(u) = u^2$ (quadratic), then the integral yields

$$\int_0^1 f((1-\xi)u_n + \xi u_{n+1})\, d\xi = \frac{u_{n+1}^2 + u_{n+1}u_n + u_n^2}{3},$$

and the AVF scheme (1.13) becomes

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{u_{n+1}^2 + u_{n+1}u_n + u_n^2}{3}. \tag{1.15}$$

If $f(u) = u^3$ (cubic), then the integral gives

$$\int_0^1 f((1-\xi)u_n + \xi u_{n+1})\, d\xi = \frac{u_{n+1}^3 + u_{n+1}^2 u_n + u_{n+1}u_n^2 + u_n^3}{4},$$

and the AVF scheme (1.13) becomes

$$\frac{u_{n+1} - u_n}{\Delta t} = \frac{u_{n+1}^3 + u_{n+1}^2 u_n + u_{n+1}u_n^2 + u_n^3}{4}. \tag{1.16}$$

AVF method is a discrete gradient method. The use of discrete gradient method has advantage for the vector field of the form

$$f(u) = S(u)\nabla V(u)$$

where $S(u)$ is a skew–symmetric matrix. For Hamiltonian system $f(u) = S(u)\nabla H(u)$ where H is the energy. When we apply the AVF method to the Hamiltonian system, the energy conservation of the numerical solution is guaranteed at each step for any choice of the integration step–size [17, 18].

To verify the order of the convergence of the average vector field method (1.13), we consider the simple harmonic oscillator problem (1.3)

$$\frac{d^2x}{dt^2} + x = 0 \tag{1.17}$$

with the initial conditions

$$x(0) = x'(0) = 1. \tag{1.18}$$

Writing the equation (1.17) as a first–order system of differential equations (see Eq. (1.5)), one can apply the average vector field method (1.13) to each equation in (1.5). The equation (1.17) together with the initial conditions (1.18) has the exact solution $x(t) = \cos(t) + \sin(t)$. We solved the problem on the region $(t, x) \in [0, 1] \times [0, 2]$. We choose the step size $\Delta t = 5.0 \times 10^{-3}$ to minimize the error. The error in this numerical calculations is measured as

$$||e_n||_\infty = \max_n |u(x_j, t_n) - u_j^n|. \tag{1.19}$$

Table 1.1 provides the results for different Δt values. We see that decreasing the temporal step size leads to decrease in the error. From the table, it can be seen that the scheme has second order convergence, where the order is calculated by

$$\text{order} \approx \ln(||e_n(\Delta t_2)||/||e_n(\Delta t_1)||)/\ln(\Delta t_2/\Delta t_1). \tag{1.20}$$

Table 1.1: Rate of convergence of the average vector field scheme (1.13).

Δt	$\|\|e_n\|\|_\infty$	order
0.1	2.501×10^{-4}	-
0.05	6.268×10^{-5}	1.996
0.025	1.568×10^{-5}	1.999
0.010	2.509×10^{-6}	1.999
0.005	6.274×10^{-7}	1.999

Although no RK method preserves polynomial invariants in general, replacing the integral in (1.13) by a quadrature, Celledoni et.al.[20] showed that there exists a RK method that preserves polynomials of any order if the polynomial is the energy invariant of a canonical Hamiltonian system. A modification of collocation methods extending the AVF method to higher order is proposed in [21]. It was shown that the new method exactly preserves polynomial or non-polynomial energy for Hamiltonian systems. Symmetry and conjugate–symplecticity of the new integrator have also been discussed. An extension of the AVF method (1.13) to the non–canonical Hamiltonian system of the form

$$\frac{du}{dt} = J(u)\nabla H(u), \quad y(t_0) = y_0 \tag{1.21}$$

has been discussed and a new class of numerical integrator is proposed in [22]. The most simple one is

$$\frac{u_{n+1} - u_n}{\Delta t} = J\left(\frac{u_{n+1} + u_n}{2}\right) \int_0^1 \nabla H((1-\xi)u_n + \xi u_{n+1})\, d\xi.$$

In [23], the AVF scheme (1.13) is applied to Hamiltonian partial differential equations (PDEs) with constant symplectic structure. The method is then applied to some PDEs in bi-Hamiltonian form with non constant Poisson structures in [24].

1.2 Nonlinear Schrödinger Equation

The single cubic nonlinear Schrödinger equation (NLS)

$$i\frac{\partial \psi(t,x)}{\partial t} + \frac{\partial^2 \psi(t,x)}{\partial x^2} + a|\psi(t,x)|^2 \psi(t,x) = 0, \tag{1.22}$$

arise in many applications such as nonlinear optics [25], biology [26], quantum mechanics [27], and hydrodynamics [28]. In the equation (1.22), $\psi(t,x)$ represents the wave function at the state point x and the time $t \in \mathbb{R}^+$. The constant a is a real parameter. In quantum mechanics $|\psi(t,x)|^2$ represents the probability density of the system at the state x and the time t [29]. The cubic nonlinearity $|\psi(t,x)|^2\psi(t,x)$ arises in the simulation of Bose-Einstein condensates [30]. The NLS equation (1.22) has infinite number of conserved quantities [31]. For example, the associated Hamiltonian energy is defined by

$$H(t) = \int_{-\infty}^{\infty} \left(\left| \frac{\partial \psi}{\partial x} \right|^2 - \frac{a}{2} |\psi|^4 \right) dx. \tag{1.23}$$

The energy is preserved in time; meaning that for all time t, we have

$$H(t) = H(0).$$

Two other conserved quantities are the mass (or charge)

$$Q(t) = \int_{-\infty}^{\infty} |\psi|^2 dx \;=\; Q(0) \tag{1.24}$$

and the momentum

$$P(t) = \int_{-\infty}^{\infty} \psi\overline{\psi_x} dx \;=\; P(t). \tag{1.25}$$

In principal, the NLS equation (1.22) can be solved by using inverse scattering transform [2, 32]. However, the corresponding solution is a special solution known as soliton solutions. They are not exact solutions. Various numerical techniques were proposed in the literature for the NLS equation (1.22) such as finite element method [33, 34], spectral method [35] and finite difference method [36]. In the last three decades, extensive numerical effort has been devoted to construct conservative schemes for NLS equation (1.22) [37]. A conservative scheme is a numerical method that preserve the discrete analog of the conserved quantities such as energy (1.23) and mass (1.24) for the NLS equation (1.22). By extensive numerical experiments, it has been shown that conservative schemes can perform better than the non–conservative schemes, and prevent the nonlinear blow–up when the discretization is fine enough [38].

In [39], a new energy-preserving method has been constructed for NLS equation based on Fourier pseudo–spectral discretization in space and the average vector field method in time. In [40] an explicit scheme, Hopscotch method, Ablowitz Ladik scheme, Crank Nicolson implicit scheme, split step Fourier method and pseudo–spectral (Fourier) method have been introduced for the numerical solution of the NLS equation. Some other conservative schemes have been developed in [6, 37, 41]. A new six point scheme based on multisymplectic formulation was presented in [42]. A relaxation scheme that preserves both mass in (1.24) and energy in (1.23) was proposed in [43]. Several geometric integrators were developed by symplectic and multisymplectic integration in [31, 44, 45]. Fei et al. [46] proposed

$$\begin{aligned} i\frac{\psi_j^{n+1} - \psi_j^{n-1}}{2\Delta t} \;=\; & \frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} - \psi_{j-1}^{n+1} + \psi_{j+1}^{n-1} - 2\psi_j^{n-1} + \psi_{j-1}^{n-1}}{2\Delta x^2} \\ & -\tfrac{a}{2}|\psi_j^n|^2 \left(\psi_j^{n+1} + \psi_j^{n-1}\right). \end{aligned} \tag{1.26}$$

as a conservative scheme for (1.22). It has been shown that the scheme (1.26) has constant energy and mass given by

$$\begin{aligned} E^n \;&=\; \sum_j \frac{\Delta x}{2}\left(\left|\frac{\psi_{j+1}^{n+1} - \psi_j^{n+1}}{\Delta x}\right|^2 + \left|\frac{\psi_{j+1}^{n} - \psi_j^{n}}{\Delta x}\right|^2\right) + \frac{a}{2}\sum_j h|\psi_j^{n+1}|^2|\psi_j^n|^2 \\ Q^n \;&=\; = \sum_j \frac{\Delta x}{2}\left(|\psi_j^n|^2 + |\psi_j^{n+1}|^2\right), \end{aligned} \tag{1.27}$$

which are the discrete analogs of the conserved quantities (1.23) and (1.24).

1.3 Two Coupled Nonlinear Schrödinger Equation

If there are two modes for describing the dynamics of slowly varying wave packets in nonlinear optics and fluid dynamics, then the coupled nonlinear Schrödinger (CNLS) equations is the relevant model. It models several physical phenomena for optical fiber, fluid dynamics representing the beam propagation in water wave interaction, the pulse propagation for fiber communication system and soliton switch in birefringent optical fibers (see [47] and reference therein). The CNLS equation

$$\begin{aligned} i\frac{\partial\psi_1}{\partial t} + \frac{\partial^2\psi_1}{\partial x^2} + \left(|\psi_1|^2 + \beta|\psi_2|^2\right)\psi_1 &= 0, \\ i\frac{\partial\psi_2}{\partial t} + \frac{\partial^2\psi_2}{\partial x^2} + \left(\beta|\psi_1|^2 + |\psi_2|^2\right)\psi_2 &= 0, \end{aligned} \tag{1.28}$$

is a mathematical model for two interacting nonlinear wave packets in a conservative and dispersive system [48]. In equation (1.28), $\psi_1(t, x)$ and $\psi_2(t, x)$ are the complex wave amplitudes, $i = \sqrt{-1}$ is the imaginary number and β is the constant which represents cross-phase modulation. If $\beta = 0$, then the equation (1.28) is reduced to two uncoupled single cubic NLS equation (1.22). The CNLS system (1.28) have admits several conserved quantities under suitable boundary conditions, such as periodic boundary conditions.

$$\frac{1}{2}\int_{-\infty}^{\infty}\left(-\left|\frac{\partial\psi_1}{\partial x}\right|^2 - \left|\frac{\partial\psi_2}{\partial x}\right|^2 + \frac{1}{2}\left(|\psi_1|^4 + |\psi_2|^4\right) + \beta|\psi_1|^2|\psi_2|^2\right)dx = \text{const}, \tag{1.29}$$

$$\int_{-\infty}^{\infty}\left(|\psi_1|^2 + |\psi_2|^2\right)dx = \text{const}, \tag{1.30}$$

$$\int_{-\infty}^{\infty} Im(\overline{\psi_1}\psi_{1x} + \overline{\psi_{2x}}\psi_2)dx = \text{const}. \tag{1.31}$$

Here, (1.29) is the energy conservation law, (1.30) is the mass/charge conservation law and (1.31) is the momentum conservation law, respectively.

In recent years, the CNLS system (1.28) has been studied numerically by several authors. In [49], a mass conserving finite difference method has been introduced. In [50] a third order exponential time differencing Runge-Kutta (ETD3RK) scheme based on $(1, 2)$ Pade approximation to exponential function has been presented for the numerical solution of CNLS equation. In [51], multisymplectic schemes are proposed. A symplectic scheme and a multisymplectic six point scheme which is equivalent to Preissman scheme are derived to investigate the periodic waves [52] and the solitary wave solution [53] of the CNLS system. In [54], a conservative finite element Galerkin method is studied. In [55], the CNLS system is simulated by using a fourth order explicit Runge-Kutta method. Fourier pseudospectral method and wavelet collocation method are also applied to the CNLS system [56]. Following the conservative scheme (1.26) for NLS equation (1.22), Ismail et.al [57] proposed the linearly implicit conservative finite difference scheme

$$\begin{aligned}
i\frac{\psi_{1,j}^{n+1}-\psi_{1,j}^{n-1}}{2\Delta t} &+ \delta_x^2\left(\frac{\psi_{1,j}^{n+1}+\psi_{1,j}^{n-1}}{2\Delta x^2}\right) + f_1(\psi_{1,j}^n,\psi_{2,j}^n)\frac{\psi_{1,j}^{n+1}+\psi_{1,j}^{n-1}}{2} = 0,\\
i\frac{\psi_{2,j}^{n+1}-\psi_{2,j}^{n-1}}{2\Delta t} &+ \delta_x^2\left(\frac{\psi_{2,j}^{n+1}+\psi_{2,j}^{n-1}}{2\Delta x^2}\right) + f_2(\psi_{1,j}^n,\psi_{2,j}^n)\frac{\psi_{2,j}^{n+1}+\psi_{2,j}^{n-1}}{2} = 0,
\end{aligned} \tag{1.32}$$

where

$$\begin{aligned}
\delta_x^2\psi_j^n &= \psi_{j+1}^n - 2\psi_j^n + \psi_{j+1}^2,\\
f_1(\psi_1,\psi_2) &= \left(|\psi_1|^2 + e|\psi_2|^2\right),\\
f_2(\psi_1,\psi_2) &= \left(e|\psi_1|^2 + |\psi_2|^2\right).
\end{aligned}$$

It has been shown that the scheme (1.32) is conservative in the sense that

$$\begin{aligned}
\sum_j \left(|\psi_{1,j}^{n+1}|^2 + |\psi_{1,j}^n|^2\right) &= \sum_j \left(|\psi_{1,j}^n|^2 + |\psi_{1,j}^{n-1}|^2\right),\\
\sum_j \left(|\psi_{2,j}^{n+1}|^2 + |\psi_{2,j}^n|^2\right) &= \sum_j \left(|\psi_{2,j}^n|^2 + |\psi_{2,j}^{n-1}|^2\right).
\end{aligned} \tag{1.33}$$

CHAPTER 2

THREE COUPLED NONLINEAR SCHRÖDINGER EQUATION

The N-coupled nonlinear Schrödinger equation (N-CNLSE) is one of the most important models which is relevant in some branches of mathematics, engineering and science. It is widely used in different fields of modern physics such as quantum mechanics [27], fluid dynamics [28] and nonlinear optics [58]. The N-CNLSE is a nonlinear partial differential equation system with second order dispersion and cubic nonlinearity defined as [59]

$$\begin{aligned}
i\frac{\partial\psi_1}{\partial t} &+ \alpha_1\frac{\partial^2\psi_1}{\partial x^2} + \left(\sigma_{11}|\psi_1|^2 + \sigma_{12}|\psi_2|^2 + \cdots + \sigma_{1N}|\psi_N|^2\right)\psi_1 = 0,\\
i\frac{\partial\psi_2}{\partial t} &+ \alpha_2\frac{\partial^2\psi_2}{\partial x^2} + \left(\sigma_{21}|\psi_1|^2 + \sigma_{22}|\psi_2|^2 + \cdots + \sigma_{2N}|\psi_N|^2\right)\psi_2 = 0,\\
&\vdots\\
i\frac{\partial\psi_N}{\partial t} &+ \alpha_N\frac{\partial^2\psi_N}{\partial x^2} + \left(\sigma_{N1}|\psi_1|^2 + \sigma_{N2}|\psi_2|^2 + \cdots + \sigma_{NN}|\psi_N|^2\right)\psi_N = 0,
\end{aligned} \tag{2.1}$$

where $\psi_n(t,x),\ n = 1,\ldots,N$ are complex functions which, in application, describe the amplitude of the wave, $\alpha_n,\ n = 1,\ldots,N$ are the dispersion coefficients and $\sigma_{jn},\ j \neq n$ are coupling parameters.

There are several theoretical and numerical studies for the $N-$CNLS equation with $N \geq 3$. In [60], exact bright one soliton and two soliton solutions for $\alpha_j = 1,, j = 1,2,3$ and $\sigma = e$ have been obtained and some shape changing collisions have been given. In [61], a new six–point scheme which is equivalent to the multisymplectic Preissman scheme have been derived for (2.1) with $N = 3$. In addition, a new periodic wave solution of 3-CNLS equation has been obtained and its stability analysis has been discussed. In [62], various split step spectral (SSSP) schemes have been presented for N-coupled nonlinear Schrödinger equation (2.1) with $N = 3,4$. In [63], a semi-explicit multisymplectic splitting scheme has been proposed to solve the system (2.1) with $N = 3$. In [64], a new central difference and quartic spline approximation based on exponential time differencing Crank-Nicolson ETD-CN method has been used for the numerical solution of (2.1) with $N \leq 3$. In [50], a new version of the Cox and Matthews' third order exponential time differencing Runge-Kutta (ETD3RK) scheme based on the (1,2)-Padé approximation to the exponential function has been introduced and some numerical results have been presented for (2.1) with $N = 2$ and 4.

The N–CNLS equation with $N = 3$ has some conserved quantities; namely, energy conservation and the mass conservation. All of the numerical methods given above for $N = 3$ ignore the energy and mass conservation of the N–CNLS equation with $N = 3$. The aim of this thesis is to construct conservative schemes that preserves energy and/or mass for N–CNLS with $N = 3$. In the following section, we will find energy and mass conservation properties of the N–CNLS equation with $N = 3$.

2.1 Conserved Quantities of 3−CNLS equations

In this thesis we will consider the following 3–coupled nonlinear Schrödinger equation

$$\begin{aligned}
i\frac{\partial\psi_1}{\partial t} &+ \alpha_1\frac{\partial^2\psi_1}{\partial x^2} + \left(\sigma|\psi_1|^2 + e|\psi_2|^2 + \sigma|\psi_3|^2\right)\psi_1 = 0,\\
i\frac{\partial\psi_2}{\partial t} &+ \alpha_2\frac{\partial^2\psi_2}{\partial x^2} + \left(e|\psi_1|^2 + \sigma|\psi_2|^2 + e|\psi_3|^2\right)\psi_2 = 0,\\
i\frac{\partial\psi_3}{\partial t} &+ \alpha_3\frac{\partial^2\psi_3}{\partial x^2} + \left(\sigma|\psi_1|^2 + e|\psi_2|^2 + \sigma|\psi_3|^2\right)\psi_3 = 0
\end{aligned} \tag{2.2}$$

in the domain

$$\Omega = \{(x,t) : x_L \le x \le x_R, \quad 0 \le t \le T\},$$

with initial conditions

$$\psi_k(x,0) = \psi_{k0}(x), \qquad k = 1,2,3, \tag{2.3}$$

and periodic boundary conditions

$$\psi_k(x_L,t) = \psi_k(x_R,t), \qquad k = 1,2,3, \tag{2.4}$$

or the homogenous boundary conditions

$$\psi_k(x_L,t) = 0, \qquad \psi_k(x_R,t) = 0, \qquad k = 1,2,3. \tag{2.5}$$

Using

$$\begin{aligned}
&\psi_1(x,t) = a(x,t) + ib(x,t), \quad \psi_2(x,t) = u(x,t) + iv(x,t),\\
&\psi_3(x,t) = p(x,t) + iq(x,t)
\end{aligned} \tag{2.6}$$

we can write (2.2) as

$$\begin{aligned}
i(a_t + ib_t) + \alpha_1(a_{xx} + ib_{xx}) + [\sigma(a^2+b^2) + e(p^2+q^2) + \sigma(u^2+v^2)](a+ib) &= 0,\\
i(p_t + iq_t) + \alpha_2(p_{xx} + iq_{xx}) + [e(a^2+b^2) + \sigma(p^2+q^2) + e(u^2+v^2)](p+iq) &= 0,\\
i(u_t + iv_t) + \alpha_3(u_{xx} + iv_{xx}) + [\sigma(a^2+b^2) + e(p^2+q^2) + \sigma(u^2+v^2)](u+vi) &= 0,
\end{aligned} \tag{2.7}$$

and decomposing the real and imaginary parts we get the real–valued system of equations

$$\begin{aligned}
a_t &+ \alpha_1 b_{xx} &+ [\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)]b &= 0,\\
p_t &+ \alpha_2 q_{xx} &+ [e(a^2+b^2)+\sigma(p^2+q^2)+e(u^2+v^2)]q &= 0,\\
u_t &+ \alpha_3 v_{xx} &+ [\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)]v &= 0,\\
b_t &- \alpha_1 a_{xx} &- [\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)]a &= 0,\\
q_t &- \alpha_2 p_{xx} &- [e(a^2+b^2)+\sigma(p^2+q^2)+e(u^2+v^2)]p &= 0,\\
v_t &- \alpha_3 u_{xx} &- [\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)]u &= 0.
\end{aligned} \tag{2.8}$$

Now, we investigate the qualitative properties of the solution of the 3-CNLS equation (2.2). In particular, we derive certain a priori bounds involving the integral invariants associated with the equation (2.2). The equation (2.2) has the following solution properties:

Theorem 2.1.1 *The solution of the* 3*-CNLS equation (2.2) satisfies the mass conservations*

$$\begin{aligned}
Q_1(t) &= \int_{x_L}^{x_R} |\psi_1(x,t)|^2\,dx = \int_{x_L}^{x_R} |\psi_1(x,0)|^2\,dx = Q_1(0),\\
Q_2(t) &= \int_{x_L}^{x_R} |\psi_2(x,t)|^2\,dx = \int_{x_L}^{x_R} |\psi_2(x,0)|^2\,dx = Q_2(0),\\
Q_3(t) &= \int_{x_L}^{x_R} |\psi_3(x,t)|^2\,dx = \int_{x_L}^{x_R} |\psi_3(x,0)|^2\,dx = Q_3(0).
\end{aligned} \tag{2.9}$$

Proof. To prove the first conservation

$$Q_1(t) = \int_{x_L}^{x_R} |\psi_1(x,t)|^2\,dx = \int_{x_L}^{x_R} |\psi_1(x,0)|^2\,dx = Q_1(0)$$

in (2.9), we decompose the real and imaginary parts of the first equation in (2.2) and get

$$i(a_t+ib_t)+\alpha_1\,(a_{xx}+ib_{xx})+\left[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)\right](a+ib)=0. \tag{2.10}$$

Taking complex conjugate of (2.10);

$$-i(a_t-ib_t)+\alpha_1\,(a_{xx}-ib_{xx})+\left[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)\right](a-ib)=0. \tag{2.11}$$

Multiplying (2.10) by $a-bi$ and multiply (2.11) by $-(a+bi)$ and add them up to get

$$i\,[(a_t+ib_t)(a-ib)+(a_t-ib_t)(a+ib)]+\alpha_1\,[(a-ib)(a_{xx}+ib_{xx})-(a+ib)(a_{xx}-ib_{xx})]=0. \tag{2.12}$$

Taking the integral of (2.12) from x_L to x_R with respect to x;

$$i\int_{x_L}^{x_R}\frac{\partial}{\partial t}\,[(a+ib)(a-ib)]\,dx+\alpha_1\int_{x_L}^{x_R}[(a-ib)(a_{xx}+ib_{xx})-(a+ib)(a_{xx}-ib_{xx})]\,dx=0.$$

Under the periodic boundary conditions (2.4) or the homogenous boundary conditions (2.5), the second integral vanishes, i.e.

$$\alpha_1\int_{x_L}^{x_R}[(a-ib)(a_{xx}+ib_{xx})-(a+ib)(a_{xx}-ib_{xx})]\,dx=0,$$

by using integration by parts. Therefore, it remains

$$\frac{\partial}{\partial t}\int_{x_L}^{x_R}(a+ib)(a-ib)dx = 0$$

that is

$$\int_{x_L}^{x_R}(a^2+b^2)dx = \int_{x_L}^{x_R}|\psi_1(x,t)|^2\,dx = \text{ const.}$$

This proves the first result in (2.9).

Second and third conservation properties in (2.9) can be shown similarly. □

Theorem 2.1.2 *The solution of the* 3*-CNLS equation (2.2) satisfies the energy conservation*

$$\begin{aligned}\mathcal{H}(t) &= \frac{1}{2}\int_{-\infty}^{\infty}\left\{-\alpha_1\left|\frac{\partial\psi_1}{\partial x}\right|^2-\alpha_2\left|\frac{\partial\psi_2}{\partial x}\right|^2-\alpha_3\left|\frac{\partial\psi_3}{\partial x}\right|^2\right.\\ &\qquad +e\,|\psi_1|^2\,|\psi_2|^2+\sigma\,|\psi_1|^2\,|\psi_3|^2+e\,|\psi_2|^2\,|\psi_3|^2 \\ &\qquad \left.+\frac{\sigma}{2}\left(|\psi_1|^4+|\psi_2|^4+|\psi_3|^4\right)\right\}dx \;=\mathcal{H}(0).\end{aligned} \tag{2.13}$$

Proof. To prove the energy conservation, we write the real and imaginary parts of the first equation in (2.2)

$$i(a_t+ib_t)+\alpha_1\,(a_{xx}+ib_{xx})+\left[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)\right](a+ib)=0. \tag{2.14}$$

Taking complex conjugate of (2.14) to get

$$-i(a_t-ib_t)+\alpha_1\,(a_{xx}-ib_{xx})+\left[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)\right](a-ib)=0. \tag{2.15}$$

Multiplying (2.14) by (a_t-ib_t) to obtain

$$\begin{aligned}&i(a_t-ib_t)(a_t+ib_t)+\alpha_1\,\{(a_t-ib_t)(a_{xx}+ib_{xx})\}\\ &\qquad +[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)](a+ib)(a_t-ib_t)=0.\end{aligned} \tag{2.16}$$

and multiplying (2.15) by (a_t+ib_t) we get

$$\begin{aligned}&-i(a_t-ib_t)(a_t+ib_t)+\alpha_1\,\{(a_t+ib_t)(a_{xx}-ib_{xx})\}\\ &\qquad +[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)](a-ib)(a_t+ib_t)=0.\end{aligned} \tag{2.17}$$

Adding (2.16) to (2.17) to get

$$\begin{aligned}&\alpha_1\,\{(a_{xx}+ib_{xx})(a_t-ib_t)+(a_{xx}-ib_{xx})(a_t+ib_t)\}\\ &\qquad +\left[\sigma(a^2+b^2)+e(p^2+q^2)+\sigma(u^2+v^2)\right]((a+ib)(a_t-ib_t)+(a-ib)(a_t+ib_t))=0.\end{aligned} \tag{2.18}$$

Integrating this result from x_L to x_R with respect to x gives

$$\alpha_1 \int_{x_L}^{x_R} \{(a_{xx} + ib_{xx})(a_t - ib_t) + (a_{xx} - ib_{xx})(a_t + ib_t)\}\, dx$$
$$+ \int_{x_L}^{x_R} [\sigma(a^2 + b^2) + e(p^2 + q^2) + \sigma(u^2 + v^2)] \frac{\partial}{\partial t} ((a + ib)(a - ib))\, dx = 0. \quad (2.19)$$

If we use integration by parts for the first integral in (2.19), then (2.19) turns out that

$$\alpha_1 [(a_t - ib_t)(a_x + ib_x) + (a_t + ib_t)(a_x - ib_x)] \Big|_{x_L}^{x_R}$$
$$- \alpha_1 \int_{x_L}^{x_R} [(a_x + ib_x)(a_{xt} - ib_{xt}) + (a_{xt} + ib_{xt})(a_x - ib_x)]$$
$$+ \int_{x_L}^{x_R} [\sigma(a^2 + b^2) + e(p^2 + q^2) + \sigma(u^2 + v^2)] \frac{\partial}{\partial t} (\left|a^2 + b^2\right|)^2 dx = 0. \quad (2.20)$$

In (2.20)

$$\alpha_1 [(a_t - ib_t)(a_x + ib_x) + (a_t + ib_t)(a_x - ib_x)] \Big|_{x_L}^{x_R} = 0$$

under the periodic boundary conditions (2.4) or the homogenous boundary conditions (2.5). Then (2.20) reduces to

$$-\alpha_1 \int_{xL}^{xR} \frac{\partial}{\partial t}(a_x^2 + b_x^2) dx + \int_{x_L}^{x_R} [\sigma(a^2 + b^2) + e(p^2 + q^2) + \sigma(u^2 + v^2)] \frac{\partial}{\partial t}(a^2 + b^2) dx = 0. \quad (2.21)$$

Following the same steps for the second and third equations in (2.2), we arrive

$$-\alpha_2 \int_{x_L}^{x_R} \frac{\partial}{\partial t}(p_x^2 + q_x^2) dx + \int_{x_L}^{x_R} [e(a^2 + b^2) + \sigma(p^2 + q^2) + e(u^2 + v^2)] \frac{\partial}{\partial t}(p^2 + q^2) dx = 0, \quad (2.22)$$

$$-\alpha_3 \int_{xL}^{xR} \frac{\partial}{\partial t}(u_x^2 + v_x^2) dx + \int_{x_L}^{x_R} [\sigma(a^2 + b^2) + e(p^2 + q^2) + \sigma(u^2 + v^2)] \frac{\partial}{\partial t}(u^2 + v^2) dx = 0. \quad (2.23)$$

Adding (2.21), (2.22) and (2.23) together, and using the equality

$$\sigma(a^2 + b^2) \frac{\partial}{\partial t}(a^2 + b^2) = \frac{\sigma}{2} \frac{\partial}{\partial t}(a^2 + b^2)^2$$

we get

$$\int_{x_L}^{x_R} \frac{\partial}{\partial t}(-\alpha_1(a_x^2 + b_x^2) - \alpha_2(p_x^2 + q_x^2) - \alpha_3(u_x^2 + v_x^2))$$
$$+ \frac{\sigma}{2} \left[\frac{\partial}{\partial t}(a_x^2 + b_x^2)^2 + (p_x^2 + q_x^2)^2 + (u_x^2 + v_x^2)^2 \right]$$
$$+ e \frac{\partial}{\partial t}(a^2 + b^2)(p^2 + q^2) + \sigma \frac{\partial}{\partial t}(a^2 + b^2)(u^2 + v^2) + e \frac{\partial}{\partial t}(p^2 + q^2)(u^2 + v^2) dx = 0.$$

i.e.

$$\frac{\partial}{\partial t} \int_{x_L}^{x_R} -\alpha_1(a_x^2 + b_x^2) - \alpha_2(p_x^2 + q_x^2) - \alpha_3(u_x^2 + v_x^2)$$
$$+ \frac{\sigma}{2} \left[(a_x^2 + b_x^2)^2 + (p_x^2 + q_x^2)^2 + (u_x^2 + v_x^2)^2 \right]$$
$$+ e \left[(a^2 + b^2)(p^2 + q^2) \right] + \sigma \left[(p^2 + q^2)(u^2 + v^2) \right] + e \left[(a^2 + b^2)(u^2 + v^2) \right] dx = 0.$$

Therefore,

$$
\int_{x_L}^{x_R} -\alpha_1(a_x^2 + b_x^2) - \alpha_2(p_x^2 + q_x^2) - \alpha_3(u_x^2 + v_x^2)
+ \frac{\sigma}{2}\Big[(a_x^2 + b_x^2)^2 + (p_x^2 + q_x^2)^2 + (u_x^2 + v_x^2)^2\Big]
+ e\Big[(a^2 + b^2)(p^2 + q^2)\Big] + \sigma\Big[(p^2 + q^2)(u^2 + v^2)\Big] + e(\Big[a^2 + b^2)(u^2 + v^2)\Big]\, dx = \text{ const;}
$$

which proves the conservation law (2.13). □

CHAPTER 3

NUMERICAL METHODS FOR 3–CNLS EQUATION

In this chapter, we will propose three different numerical methods for the solution of the 3–CNLS equation (2.2) and discuss their properties in terms of conservation of mass (2.9) and energy (2.13).

3.1 Average Vector Field Method for 3-CNLS equation

In this section, we will propose an energy preserving numerical method by using average vector field method for 3-CNLS equation (2.2).

We start by writing the 3−CNLS equation (2.8), as the infinite dimensional Hamiltonian form

$$\mathbf{z}_t = \mathcal{S}\left(\frac{\delta}{\delta \mathbf{z}}\right)\mathcal{H}\,(\mathbf{z}), \tag{3.1}$$

where $\mathbf{z} = (a, p, u, b, q, v)^T$ with the skew-symmetric matrix $\mathcal{S}$

$$\mathcal{S} = \begin{pmatrix} \mathbf{0} & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{pmatrix},$$

where $\mathbf{0}$ is the zero matrix and $\mathbf{I}$ is the identity matrix with dimension 3×3. The variational derivative is given by [65]

$$\frac{\delta \mathcal{H}}{\delta \mathbf{z}} = \frac{\partial H}{\partial \mathbf{z}} - \partial_x\left(\frac{\partial H}{\partial \mathbf{z}_x}\right) + \partial_{xx}\left(\frac{\partial H}{\partial \mathbf{z}_{xx}}\right) - \cdots,$$

where

$$\mathcal{H}(z) = \int H(\mathbf{z}, \mathbf{z}_x)dx. \tag{3.2}$$

$\mathcal{H}$ is the Hamiltonian for the system (2.2) defined in (2.13).

We consider the 3−CNLS equation (2.2) with the initial conditions (2.3) and the periodic boundary conditions (2.4). For approximating this problem, we introduce the following spatial discretization

$$x_j = x_L + j\Delta x,\ j = 0, 1, 2 \ldots M, \quad \Delta x = \frac{x_R - x_L}{M}$$

and temporal discretization

$$t_n = n\Delta t, n = 1, 2, \ldots N, \quad \frac{T}{N}$$

where $\Delta x > 0$ and $\Delta t > 0$ are fixed space step and time step, respectively. The points in the domain $[x_L, x_R] \times [0, T]$ define a regular grid (or mesh) in two dimensions. We use the vectors

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_M \end{pmatrix}, \qquad \psi = \begin{pmatrix} \psi_1(t) \\ \vdots \\ \psi_M(t) \end{pmatrix}$$

with

$$\psi_j(t) \approx \psi(x_j, t).$$

Since we use periodic boundary conditions, we also set

$$\psi_{M+1} \equiv \psi_1(t), \quad \psi_0(t) \equiv \psi_M(t), \qquad t > 0.$$

The second order spatial derivative is discretized by

$$\frac{\partial^2 \psi}{\partial x^2} \approx \frac{\psi_{j-1} - 2\psi_j + \psi_{j+1}}{\Delta x^2}, \quad j = 1, \cdots, M.$$

Then the system of equations in (2.8) yield the following semi–discrete problem

$$\begin{aligned}
\frac{da_j}{dt} &= -\alpha_1 \frac{b_{j-1} + 2b_j + b_{j+1}}{\Delta x^2} + S_{1,j} b_j, \\
\frac{dp_j}{dt} &= -\alpha_2 \frac{q_{j-1} + 2q_j + q_{j+1}}{\Delta x^2} + S_{2,j} q_j \\
\frac{du_j}{dt} &= -\alpha_3 \frac{v_{j-1} + 2v_j + v_{j+1}}{\Delta x^2} + S_{1,j} v_j, \\
\frac{db_j}{dt} &= \alpha_1 \frac{a_{j-1} + 2a_j + a_{j+1}}{\Delta x^2} + S_{1,j} a_j, \\
\frac{dq_j}{dt} &= \alpha_2 \frac{p_{j-1} + 2p_j + p_{j+1}}{\Delta x^2} + S_{2,j} p_j, \\
\frac{dv_j}{dt} &= \alpha_3 \frac{u_{j-1} + 2u_j + u_{j+1}}{\Delta x^2} + S_{1,j} u_j,
\end{aligned} \tag{3.3}$$

where

$$S_{1,j} = \sigma(a_j^2 + b_j^2) + e(p_j^2 + q_j^2) + \sigma(u_j^2 + v_j^2)$$

and

$$S_{2,j} = e(a_j^2 + b_j^2) + \sigma(p_j^2 + q_j^2) + e(u_j^2 + v_j^2).$$

This is a nonlinear system of $6M$ equations with $6M$ unknowns $(\mathbf{a_j}, \mathbf{b_j}, \mathbf{p_j}, \mathbf{q_j}, \mathbf{u_j}, \mathbf{v_j})^T$, $j = 1, 2, \ldots, M$.

To understand the structure of the above system, we write the first equation of (3.3) explicitly as

$$\begin{aligned}
\frac{da_1}{dt} &= -\alpha_1 \frac{b_M + 2b_1 + b_2}{\Delta x^2} + S_{1,1} b_1, \\
\frac{da_2}{dt} &= -\alpha_1 \frac{b_1 + 2b_2 + b_3}{\Delta x^2} + S_{1,2} b_2, \\
&\vdots \\
\frac{da_{M-1}}{dt} &= -\alpha_1 \frac{b_{M-2} + 2b_{M-1} + b_M}{\Delta x^2} + S_{1,(M-1)} b_{M-1}, \\
\frac{da_M}{dt} &= -\alpha_1 \frac{b_{M-1} + 2b_M + b_1}{\Delta x^2} + S_{1,M} b_M.
\end{aligned} \tag{3.4}$$

The other equations in (3.3) can be written similarly. The nonlinear system of equations (3.3) is a Hamiltonian system of equations. In fact, by introducing the vector $\mathbf{Z} = (\mathbf{a_j}, \mathbf{b_j}, \mathbf{p_j}, \mathbf{q_j}, \mathbf{u_j}, \mathbf{v_j})^T$, $j = 1, 2, \ldots, M$ and the $6M \times 6M$ skew–symmetric matrix

$$\mathbf{J} = \frac{1}{\Delta x} \begin{pmatrix} \mathbf{0_{3Mx3M}} & -\mathbf{I_{3Mx3M}} \\ \mathbf{I_{3Mx3M}} & \mathbf{0_{3Mx3M}}, \end{pmatrix} \tag{3.5}$$

where $\mathbf{0_{3Mx3M}}$ and $\mathbf{I_{3Mx3M}}$ are $3Mx3M$ zero and identity matrices, respectively, we can express the system of equation (3.3) as a finite dimensional Hamiltonian equation of the form

$$\frac{d\mathbf{Z}}{dt} = \mathbf{J} \nabla H(\mathbf{Z}), \tag{3.6}$$

where the Hamiltonian $H(\mathbf{Z})$ given by

$$\begin{aligned}
H(\mathbf{Z}) &= \Delta x \sum_{j=1}^{M} \frac{1}{2} \Bigg\{ -\alpha_1 \left(\frac{a_{j+1} - a_j}{\Delta x} \right)^2 - \alpha_1 \left(\frac{b_{j+1} - b_j}{\Delta x} \right)^2 \\
&-\alpha_2 \left(\frac{p_{j+1} - p_j}{\Delta x} \right)^2 - \alpha_2 \left(\frac{q_{j+1} - q_j}{\Delta x} \right)^2 \\
&-\alpha_3 \left(\frac{u_{j+1} - u_j}{\Delta x} \right)^2 - \alpha_3 \left(\frac{v_{j+1} - v_j}{\Delta x} \right)^2 \\
&+e(a_j^2 + b_j^2)(p_j^2 + q_j^2) + \sigma(a_j^2 + b_j^2)(u_j^2 + v_j^2) \\
&+e(p_j^2 + q_j^2)(u_j^2 + v_j^2) \Bigg\},
\end{aligned} \tag{3.7}$$

which is the discrete analog of the energy $\mathcal{H}(\mathbf{z})$ in (2.13).

This means that the time evolution will be generated by the Hamiltonian equations

$$\begin{aligned}
\frac{da_j}{dt} &= -\frac{1}{\Delta x}\frac{\partial H}{\partial b_j}, \quad \frac{db_j}{dt} = \frac{1}{\Delta x}\frac{\partial H}{\partial a_j}, \quad \frac{dp_j}{dt} = -\frac{1}{\Delta x}\frac{\partial H}{\partial q_j}, \\
\frac{dq_j}{dt} &= \frac{1}{\Delta x}\frac{\partial H}{\partial p_j}, \quad \frac{du_j}{dt} = -\frac{1}{\Delta x}\frac{\partial H}{\partial v_j}, \quad \frac{dv_j}{dt} = \frac{1}{\Delta x}\frac{\partial H}{\partial u_j},
\end{aligned} \tag{3.8}$$

which can be written explicitly as a matrix equation

$$\frac{d}{dt}\begin{bmatrix} a_j \\ p_j \\ u_j \\ b_j \\ q_j \\ v_j \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -\mathbf{I_{MxM}} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\mathbf{I_{MxM}} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\mathbf{I_{MxM}} \\ \mathbf{I_{MxM}} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{I_{MxM}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{I_{MxM}} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\Delta x}\frac{\partial H}{\partial a_j} \\ \frac{1}{\Delta x}\frac{\partial H}{\partial p_j} \\ \frac{1}{\Delta x}\frac{\partial H}{\partial u_j} \\ \frac{1}{\Delta x}\frac{\partial H}{\partial b_j} \\ \frac{1}{\Delta x}\frac{\partial H}{\partial q_j} \\ \frac{1}{\Delta x}\frac{\partial H}{\partial v_j} \end{bmatrix}.$$

In order to check the Hamiltonian formalism (3.6), we write (3.7) explicitly for $j = 1, 2, \ldots, M$ and obtain

$$\begin{aligned} H(\mathbf{Z}) = \frac{-\alpha_1}{2\Delta x} & \Big\{(a_2 + a_1)^2 + (a_3 + a_2)^2 + \ldots + (a_M + a_{M-1})^2 + (a_{M+1} + a_M)^2 \\ & + (b_2 + b_1)^2 + (b_3 + b_2)^2 + \ldots + (b_M + b_{M-1})^2 + (b_{M+1} + b_M)^2\Big\} \\ & - \frac{\alpha_2}{2\Delta x}\Big\{(p_2 + p_1)^2 + (p_3 + p_2)^2 + \ldots + (p_M + p_{M-1})^2 + (p_{M-1} + p_M)^2 \\ & + (q_2 + q_1)^2 + (q_3 + q_2)^2 + \ldots + (q_M + q_{M-1})^2 + (q_{M+1} + q_M)^2\Big\} \\ & - \frac{\alpha_3}{2\Delta x}\Big\{(u_2 + u_1)^2 + (u_3 + u_2)^2 + \ldots + (u_M + u_{M-1})^2 + (u_{M+1} + u_M)^2 \\ & + (v_2 + v_1)^2 + (v_3 + v_2)^2 + \ldots + (v_M + v_{M-1})^2 + (v_{M+1} + v_M)^2 + \Big\} \\ & + \frac{e\Delta x}{2}\left[\left(a_1^2 + b_1^2\right)\left(p_1^2 + q_1^2\right)\ldots\left(a_M^2 + b_M^2\right)\left(p_M^2 + q_M^2\right)\right] \\ & + \frac{\sigma\Delta x}{2}\left[\left(a_1^2 + b_1^2\right)\left(u_1^2 + v_1^2\right)\ldots\left(a_M^2 + b_M^2\right)\left(u_M^2 + v_M^2\right)\right] \\ & + \frac{e\Delta x}{2}\left[\left(p_1^2 + q_1^2\right)\left(u_1^2 + v_1^2\right)\ldots\left(p_M^2 + q_M^2\right)\left(u_M^2 + v_M^2\right)\right] \\ & + \frac{\sigma\Delta x}{4}\Big[\left(a_1^2 + b_1^2\right)^2 + \left(p_1^2 + q_1^2\right)^2 + \left(u_1^2 + v_1^2\right)^2 \\ & + \cdots + \left(a_M^2 + b_M^2\right)^2 + \left(p_M^2 + q_M^2\right)^2 + \left(u_M^2 + v_M^2\right)^2\Big]. \end{aligned} \tag{3.9}$$

In equation (3.6), the first term of the gradient $\nabla_{\mathbf{Z}} H(\mathbf{Z})$ is

$$\begin{aligned} \frac{\partial H}{\partial b_1} &= \frac{-\alpha_1}{\Delta x}\left[-(b_2 - b_1) + (b_1 - b_M)\right] + e\Delta x\left[b_1\left(p_1^2 + q_1^2\right)\right] \\ & \quad + \sigma\Delta x\left[b_1\left(u_1^2 + v_1^2\right)\right] + \sigma\Delta x\left[\left(a_1^2 + b_1^2\right)b_1\right] \\ &= \frac{\alpha_1}{\Delta x}\left[(b_2 - 2b_1 + b_M)\right] + e\Delta x\left[b_1\left(p_1^2 + q_1^2\right)\right] \\ & \quad + \sigma\Delta x\left[b_1\left(u_1^2 + v_1^2\right)\right] + \sigma\Delta x\left[\left(a_1^2 + b_1^2\right)b_1\right] \end{aligned} \tag{3.10}$$

so that the first equation of (3.6) is

$$\begin{aligned}\frac{da_1}{dt} &= \frac{-1}{\Delta x}\frac{\partial H}{\partial b_1} \\ &= \frac{-\alpha_1}{\Delta x^2}\left[(b_2 - 2b_1 + b_M)\right] - \left[\sigma\left(a_1^2 + b_1^2\right) + \ e\left(p_1^2 + q_1^2\right) + \sigma\left(u_1^2 + v_1^2\right)\right] b_1,\end{aligned}$$

which is the first equation in (3.4). The other equations can be verified similarly.

The system of ordinary differential equations (3.6) can be discretized in time by using the AVF method [23, 17],

$$\frac{\mathbf{Z}_{n+1} - \mathbf{Z}_n}{\Delta t} = \mathbf{J} \int_0^1 \nabla H((1-\xi)\mathbf{Z}_n + \xi\mathbf{Z}_{n+1})\, d\xi. \tag{3.11}$$

Equation (3.11) conserves the energy (3.7). In order to prove that the method (3.11) preserves energy, we take the scalar product with

$$\left(\int_0^1 \nabla H((1-\xi)\mathbf{Z}_n + \xi\mathbf{Z}_{n+1})\, d\xi\right)^T$$

on both sides of the equation (3.11) and get

$$\frac{1}{\Delta t}\int_0^1 (z_{n+1} - z_n)\,.\nabla H((1-\xi)\mathbf{Z}_n + \xi\mathbf{Z}_{n+1})\, d\xi = 0,$$

i.e

$$\frac{1}{\Delta t}\int_0^1 \frac{d}{d\xi} H((1-\xi)\mathbf{Z}_n + \xi\mathbf{Z}_{n+1})\, d\xi = 0. \tag{3.12}$$

Using Fundamental Theorem of Calculus, we get

$$\frac{1}{\Delta t} H((Z_{n+1}) - H(Z_n)) = 0, \tag{3.13}$$

and therefore

$$H(Z_{n+1}) = H(Z_n), \tag{3.14}$$

which means that energy is same at every time step i.e., the method conserves the energy. The existence of the above discrete energy conservation law (3.14) guarantees that the numerical scheme will not blow–up and the scheme (3.11) will be stable [46, 66].

Now, we write the equations in (3.11) explicitly to discuss the solution of this non–linear system of equations. Applying the AVF method (3.11) to each equation in (3.6), one obtains:

$$\begin{aligned}
\frac{a_j^{n+1}-a_j^n}{\Delta t} &= \frac{-1}{\Delta x}\int_0^1 \frac{\partial H}{\partial b_j}\left((1-\xi)\,a_j^n+\xi a_j^{n+1},\ldots,(1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi,\\
\frac{p_j^{n+1}-p_j^n}{\Delta t} &= \frac{-1}{\Delta x}\int_0^1 \frac{\partial H}{\partial q_j}\left((1-\xi)\,a_j^n+\xi a_j^{n+1},\ldots,(1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi,\\
\frac{u_j^{n+1}-u_j^n}{\Delta t} &= \frac{-1}{\Delta x}\int_0^1 \frac{\partial H}{\partial v_j}\left((1-\xi)\,a_j^n+\xi a_j^{n+1},\ldots,(1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi,\\
\frac{b_j^{n+1}-b_j^n}{\Delta t} &= \frac{1}{\Delta x}\int_0^1 \frac{\partial H}{\partial a_j}\left((1-\xi)\,a_j^n+\xi a_j^{n+1},\ldots,(1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi,\\
\frac{q_j^{n+1}-q_j^n}{\Delta t} &= \frac{1}{\Delta x}\int_0^1 \frac{\partial H}{\partial p_j}\left((1-\xi)\,a_j^n+\xi a_j^{n+1},\ldots,(1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi,\\
\frac{v_j^{n+1}-v_j^n}{\Delta t} &= \frac{1}{\Delta x}\int_0^1 \frac{\partial H}{\partial u_j}\left((1-\xi)\,a_j^n+\xi a_j^{n+1},\ldots,(1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi.
\end{aligned} \tag{3.15}$$

Evaluating the partial derivatives we get

$$\begin{aligned}
\frac{a_j^{n+1}-a_j^n}{\Delta t} = \int_0^1 &\frac{-\alpha_1}{\Delta x^2}\left((1-\xi)\left(b_{j-1}^n-2b_j^n+b_{j+1}^n\right)+\xi\left(b_{j-1}^{n+1}-2b_j^{n+1}+b_{j+1}^{n+1}\right)\right)\\
&-\Big\{\sigma\left[\left((1-\xi)\,a_j^n+\xi a_j^{n+1}\right)^2+\left((1-\xi)\,b_j^n+\xi b_j^{n+1}\right)^2\right]\\
&+\ e\left[\left((1-\xi)\,p_j^n+\xi p_j^{n+1}\right)^2+\left((1-\xi)\,q_j^n+\xi q_j^{n+1}\right)^2\right]\\
&+\ \sigma\left[\left((1-\xi)\,u_j^n+\xi u_j^{n+1}\right)^2+\left((1-\xi)\,v_j^n+\xi v_j^{n+1}\right)^2\right]\Big\}\left((1-\xi)\,b_j^n+\xi b_j^{n+1}\right)d\xi,
\end{aligned}$$

$$\begin{aligned}
\frac{p_j^{n+1}-p_j^n}{\Delta t} = \int_0^1 &\frac{-\alpha_2}{\Delta x^2}\left((1-\xi)\left(q_{j-1}^n-2q_j^n+b_{j+1}^n\right)+\xi\left(q_{j-1}^{n+1}-2q_j^{n+1}+q_{j+1}^{n+1}\right)\right)\\
&-\Big\{\ e\left[\left((1-\xi)\,a_j^n+\xi a_j^{n+1}\right)^2+\left((1-\xi)\,b_j^n+\xi b_j^{n+1}\right)^2\right]\\
&+\sigma\left[\left((1-\xi)\,p_j^n+\xi p_j^{n+1}\right)^2+\left((1-\xi)\,q_j^n+\xi q_j^{n+1}\right)^2\right]\\
&+\ e\left[\left((1-\xi)\,u_j^n+\xi u_j^{n+1}\right)^2+\left((1-\xi)\,v_j^n+\xi v_j^{n+1}\right)^2\right]\Big\}\left((1-\xi)\,q_j^n+\xi q_j^{n+1}\right)d\xi,
\end{aligned}$$

$$\begin{aligned}
\frac{u_j^{n+1}-u_j^n}{\Delta t} = \int_0^1 &\frac{-\alpha_3}{\Delta x^2}\left((1-\xi)\left(v_{j-1}^n-2v_j^n+v_{j+1}^n\right)+\xi\left(v_{j-1}^{n+1}-2v_j^{n+1}+v_{j+1}^{n+1}\right)\right)\\
&-\Big\{\sigma\left[\left((1-\xi)\,a_j^n+\xi a_j^{n+1}\right)^2+\left((1-\xi)\,b_j^n+\xi b_j^{n+1}\right)^2\right]\\
&+\ e\left[\left((1-\xi)\,p_j^n+\xi p_j^{n+1}\right)^2+\left((1-\xi)\,q_j^n+\xi q_j^{n+1}\right)^2\right]\\
&+\ \sigma\left[\left((1-\xi)\,u_j^n+\xi u_j^{n+1}\right)^2+\left((1-\xi)\,v_j^n+\xi v_j^{n+1}\right)^2\right]\Big\}\left((1-\xi)\,v_j^n+\xi v_j^{n+1}\right)d\xi,
\end{aligned}$$

$$\frac{b_j^{n+1}-b_j^n}{\Delta t} = \int_0^1 \frac{\alpha_1}{\Delta x^2}\left((1-\xi)\left(a_{j-1}^n - 2a_j^n + a_{j+1}^n\right) + \xi\left(a_{j-1}^{n+1} - 2a_j^{n+1} + a_{j+1}^{n+1}\right)\right)$$
$$+\left\{\sigma\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+\ e\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\ \sigma\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right) d\xi,$$

$$\frac{q_j^{n+1}-q_j^n}{\Delta t} = \int_0^1 \frac{\alpha_2}{\Delta x^2}\left((1-\xi)\left(p_{j-1}^n - 2p_j^n + p_{j+1}^n\right) + \xi\left(p_{j-1}^{n+1} - 2p_j^{n+1} + p_{j+1}^{n+1}\right)\right)$$
$$+\left\{\ e\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+\ \sigma\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\ e\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,p_j^n + p_j^{n+1}\right) d\xi,$$

and

$$\frac{v_j^{n+1}-v_j^n}{\Delta t} = \int_0^1 \frac{\alpha_3}{\Delta x^2}\left((1-\xi)\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \xi\left(u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}\right)\right)$$
$$+\left\{\sigma\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+\ e\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\ \sigma\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,u_j^n + u_j^{n+1}\right) d\xi.$$

Evaluating the integrals on the right–hand side of the equations yields $6M$ non–linear equations with $6M$ unknowns. The equations (3.15) yield $6M$ nonlinear systems of equations

$$F_{1,j} = \left(a_j^{n+1} - a_j^n\right) - \frac{\alpha_1 \Delta t}{2\Delta x^2}\left(b_{j-1}^n - 2b_j^n + b_{j+1}^n + b_{j-1}^{n+1} - 2b_j^{n+1} + b_{j+1}^{n+1}\right)$$
$$-\ \Delta t \int_0^1 \left\{\sigma\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+\ e\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\sigma\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right) d\xi,$$

$$F_{2,j} = \left(p_j^{n+1} - p_j^n\right) - \frac{\alpha_2 \Delta t}{2\Delta x^2}\left(q_{j-1}^n - 2q_j^n + b_{j+1}^n + q_{j-1}^{n+1} - 2q_j^{n+1} + q_{j+1}^{n+1}\right)$$
$$-\ \Delta t \int_0^1 \left\{e\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+\ \sigma\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+e\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right) d\xi,$$

$$F_{3,j} = \left(u_j^{n+1} - u_j^n\right) - \frac{\alpha_3 \Delta t}{2\Delta x^2}\left(v_{j-1}^n - 2v_j^n + v_{j+1}^n + v_{j-1}^{n+1} - 2v_j^{n+1} + v_{j+1}^{n+1}\right)$$
$$- \Delta t \int_0^1 \left\{\sigma\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+ e\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\sigma\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right) d\xi,$$

$$F_{4,j} = \left(b_j^{n+1} - b_j^n\right) + \frac{\alpha_1 \Delta t}{2\Delta x^2}\left(a_{j-1}^n - 2a_j^n + a_{j+1}^n + a_{j-1}^{n+1} - 2a_j^{n+1} + a_{j+1}^{n+1}\right)$$
$$+ \Delta t \int_0^1 \left\{\sigma\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+ e\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\sigma\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right) d\xi,$$

$$F_{5,j} = \left(q_j^{n+1} - q_j^n\right) + \frac{\alpha_2 \Delta t}{2\Delta x^2}\left(p_{j-1}^n - 2p_j^n + p_{j+1}^n + p_{j-1}^{n+1} - 2p_j^{n+1} + p_{j+1}^{n+1}\right)$$
$$+ \Delta t \int_0^1 \left\{ e\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+ \sigma\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+e\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,p_j^n + p_j^{n+1}\right) d\xi$$

and

$$F_{6,j} = \left(v_j^{n+1} - v_j^n\right) + \frac{\alpha_3 \Delta t}{2\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}\right)$$
$$+ \Delta t \int_0^1 \left\{\sigma\left[\left((1-\xi)\,a_j^n + \xi a_j^{n+1}\right)^2 + \left((1-\xi)\,b_j^n + \xi b_j^{n+1}\right)^2\right]\right.$$
$$+ e\left[\left((1-\xi)\,p_j^n + \xi p_j^{n+1}\right)^2 + \left((1-\xi)\,q_j^n + \xi q_j^{n+1}\right)^2\right]$$
$$\left.+\sigma\left[\left((1-\xi)\,u_j^n + \xi u_j^{n+1}\right)^2 + \left((1-\xi)\,v_j^n + \xi v_j^{n+1}\right)^2\right]\right\}\left((1-\xi)\,u_j^n + u_j^{n+1}\right) d\xi,$$

with the Jacobian matrix J

$$J = \begin{bmatrix} \frac{\partial F_{1,j}}{\partial a_j^{n+1}} & \frac{\partial F_{1,j}}{\partial b_j^{n+1}} & \frac{\partial F_{1,j}}{\partial p_j^{n+1}} & \frac{\partial F_{1,j}}{\partial q_j^{n+1}} & \frac{\partial F_{1,j}}{\partial u_j^{n+1}} & \frac{\partial F_{1,j}}{\partial v_j^{n+1}} \\ \frac{\partial F_{2,j}}{\partial a_j^{n+1}} & \frac{\partial F_{2,j}}{\partial b_j^{n+1}} & \frac{\partial F_{2,j}}{\partial p_j^{n+1}} & \frac{\partial F_{2,j}}{\partial q_j^{n+1}} & \frac{\partial F_{2,j}}{\partial u_j^{n+1}} & \frac{\partial F_{2,j}}{\partial v_j^{n+1}} \\ \frac{\partial F_{3,j}}{\partial a_j^{n+1}} & \frac{\partial F_{3,j}}{\partial b_j^{n+1}} & \frac{\partial F_{3,j}}{\partial p_j^{n+1}} & \frac{\partial F_{3,j}}{\partial q_j^{n+1}} & \frac{\partial F_{3,j}}{\partial u_j^{n+1}} & \frac{\partial F_{3,j}}{\partial v_j^{n+1}} \\ \frac{\partial F_{4,j}}{\partial a_j^{n+1}} & \frac{\partial F_{4,j}}{\partial b_j^{n+1}} & \frac{\partial F_{4,j}}{\partial p_j^{n+1}} & \frac{\partial F_{4,j}}{\partial q_j^{n+1}} & \frac{\partial F_{4,j}}{\partial u_j^{n+1}} & \frac{\partial F_{4,j}}{\partial v_j^{n+1}} \\ \frac{\partial F_{5,j}}{\partial a_j^{n+1}} & \frac{\partial F_{5,j}}{\partial b_j^{n+1}} & \frac{\partial F_{5,j}}{\partial p_j^{n+1}} & \frac{\partial F_{5,j}}{\partial q_j^{n+1}} & \frac{\partial F_{5,j}}{\partial u_j^{n+1}} & \frac{\partial F_{5,j}}{\partial v_j^{n+1}} \\ \frac{\partial F_{6,j}}{\partial a_j^{n+1}} & \frac{\partial F_{6,j}}{\partial b_j^{n+1}} & \frac{\partial F_{6,j}}{\partial p_j^{n+1}} & \frac{\partial F_{6,j}}{\partial q_j^{n+1}} & \frac{\partial F_{6,j}}{\partial u_j^{n+1}} & \frac{\partial F_{6,j}}{\partial v_j^{n+1}} \end{bmatrix}_{6Mx6M} . \tag{3.16}$$

This non–linear system of equations can be solved by using an iterative scheme such as Newton's method or fixed point iteration [67]. Here we use Newton's method

$$\begin{bmatrix} a_j^{n+1} \\ p_j^{n+1} \\ u_j^{n+1} \\ b_j^{n+1} \\ q_j^{n+1} \\ v_j^{n+1} \end{bmatrix} = \begin{bmatrix} a_j^{n} \\ p_j^{n} \\ u_j^{n} \\ b_j^{n} \\ q_j^{n} \\ v_j^{n} \end{bmatrix} - \mathbf{J_F^{-1}}\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \begin{bmatrix} F_1\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \\ F_2\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \\ F_3\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \\ F_4\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \\ F_5\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \\ F_6\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) \end{bmatrix}. \tag{3.17}$$

Newton's method for solving a non-linear system of equation $\mathbf{G}(\mathbf{x}) = 0$ uses the Jacobian matrix of $\mathbf{G}$, i.e. $\mathbf{J_G}$ at every iteration. But inverting the Jacobian matrix at every iteration is difficult and time consuming. Therefore, to find the inverse of the Jacobian matrix efficiently, first we consider the linear systems of equation by setting

$$\mathbf{J_F^{-1}}\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right)\mathbf{F}\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) = \mathbf{X}$$

in (3.17) and first solve the linear system of equation

$$\mathbf{F}\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right) = \mathbf{J_F X}$$

by using the LU decomposition of the matrix $\mathbf{J_F} = \mathbf{LU}$. Then we get

$$\mathbf{F} = (\mathbf{LU})\,\mathbf{X}, \tag{3.18}$$

where $\mathbf{L}$ and $\mathbf{U}$ are lower and upper triangular matrices, respectively. Let

$$\mathbf{Ly} = \mathbf{F} \Rightarrow \mathbf{y} = \mathbf{L}^{-1}\mathbf{F}$$

and

$$\mathbf{UX} = \mathbf{y}$$

$$\mathbf{X} = \mathbf{U}^{-1}\mathbf{y}.$$

Finally, the Newton's method (3.17) proceeds by

$$\begin{bmatrix} a_j^{n+1} \\ p_j^{n+1} \\ u_j^{n+1} \\ b_j^{n+1} \\ q_j^{n+1} \\ v_j^{n+1} \end{bmatrix} = \begin{bmatrix} a_j^{n} \\ p_j^{n} \\ u_j^{n} \\ b_j^{n} \\ q_j^{n} \\ v_j^{n} \end{bmatrix} - \mathbf{X}\left(a_j^n, \ldots, v_j^n, a_j^{n+1}, \ldots, v_j^{n+1}\right).$$

up to the error tolerance $|\mathbf{Z}^{n+1} - \mathbf{Z}^n| < tol = 10^{-7}$, where $\mathbf{Z} = (a_j, b_j, p_j, q_j, u_j, v_j)^T$.

Two iterations satisfy

$$|\mathbf{Z}^{n+1} - \mathbf{Z}^{n}| < tol$$

for $tol = 10^{-7}$. When we decrease the tolerance to $tol = 10^{-15}$, three iterations satisfy the required accuracy in Newton iteration.

3.1.1 Linear Stability Analysis

In this section, we investigate the accuracy, linear stability and truncation error of the AVF method (3.11). Although an application of the linear stability analysis to nonlinear equations cannot be justified, it is found to be effective in practice. Consider the linearized form [49] of the equation (2.2):

$$\begin{aligned} i\psi_{1_t} &+ \alpha_1\psi_{1_{xx}} &+ \overline{S}_1\psi 1 &= 0, \\ i\psi_{2_t} &+ \alpha_2\psi_{2_{xx}} &+ \overline{S}_2\psi 2 &= 0, \\ i\psi_{3_t} &+ \alpha_3\psi_{3_{xx}} &+ \overline{S}_1\psi 3 &= 0, \end{aligned} \tag{3.19}$$

where the constant terms are

$$\begin{aligned} \overline{S_1} &= \max_{x_x \le x \le x_R} \{\sigma|\psi_1| + e|\psi_2| + \sigma|\psi_3|\}, \\ \overline{S_2} &= \max_{x_x \le x \le x_R} \{e|\psi_1| + \sigma|\psi_2| + e|\psi_3|\}. \end{aligned}$$

.

Application of the AVF scheme (1.13) to the linear equation (3.19) yields the implicit midpoint rule (1.14)

$$i\frac{\psi_{k,j}^{n+1} - \psi_{k,j}^{n}}{\Delta t} + \alpha_k\delta_x^2\left(\frac{\psi_{k,j}^{n+1} + \psi_{k,j}^{n}}{2}\right) + \overline{S}\left(\frac{\psi_{k,j}^{n+1} + \psi_{k,j}^{n}}{2}\right) = 0, \tag{3.20}$$

where $\overline{S} = \overline{S_1}$ for $k = 1,3$ and $\overline{S} = \overline{S_2}$ for $k = 2$,

$$\delta_x^2\psi_j^n = \frac{1}{\Delta x^2}\left(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n\right).$$

Theorem 3.1.1 *The AVF method (3.11) for the equations (3.19) is a consistent method with the order of accuracy* $\mathcal{O}((\Delta t)^2) + \mathcal{O}((\Delta x)^2)$.

Proof. We start by assuming that the numerical method is exact at the grid point (x_j, t_n). Then the local truncation error is

$$\begin{aligned} LTE := \frac{\psi_k(x_j,t_{n+1}) - \psi_k(x_j,t_n)}{\Delta t} &+ \alpha_k\delta_x^2\left(\frac{\psi_k(x_j,t_{n+1}) + \psi_k(x_j,t_n)}{2}\right) \\ &+ \overline{S}\left(\frac{\psi_k(x_j,t_{n+1}) + \psi_k(x_j,t_n)}{2}\right), \quad k = 1,2,3. \end{aligned} \tag{3.21}$$

Taylor's series expansions of all terms in (3.20) about the grid point (t_n, x_j) can be given as follows:

The first term in (3.21):

$$\frac{\psi_{k,j}^{n+1} - \psi_{k,j}^{n}}{\Delta t} = \left(\psi_{k,t} + \frac{\Delta t}{2}\psi_{k,tt} + \frac{\Delta t^2}{6}\psi_{k,ttt} + \cdots\right); \tag{3.22}$$

The second term (3.21):

$$\frac{\alpha_1}{2}\left(\frac{\psi_{k,j-1}^{n+1} - 2\psi_{k,j}^{n+1} + \psi_{k,j+1}^{n+1}}{\Delta x^2} + \frac{\psi_{k,j-1}^{n} - 2\psi_{k,j}^{n} + \psi_{k,j+1}^{n}}{\Delta x^2}\right)$$
$$= \frac{\alpha_k}{2\Delta x^2}\left(2\psi_{k,xx}\Delta x^2 + \psi_{k,xxxx}\frac{\Delta x^4}{12} + \psi_{k,xxt}\frac{\Delta x^2\Delta t}{2} + \psi_{k,xxtt}\frac{\Delta x^2\Delta t^2}{2} + ...\right), \tag{3.23}$$

and the third term in (3.21):

$$\frac{\overline{S}}{2}\left\{\psi_{k,j}^{n+1} + \psi_{k,j}^{n}\right\} = \frac{\overline{S}}{2}\left(2\psi_k + \Delta t\psi_{k,t} + \frac{\Delta t^2}{2}\psi_{k,tt} + ...\right). \tag{3.24}$$

Substituting (3.22)-(3.24) into the equation (3.21) leads to

$$LTE = \left(\psi_{k,t} + \alpha_k\psi_{k,xx} + S_j^n\psi_k\right)$$
$$+ \frac{\Delta t}{2}\psi_{k,tt} + \frac{\Delta t^2}{6}\psi_{k,ttt} + \alpha\left(\frac{\Delta x^2}{12}\psi_{k,xxxx} + \frac{\Delta t^2}{2}\psi_{k,xxtt} + \frac{\Delta t}{2}\psi_{k,xxt}\right)$$
$$+ \overline{S}\left(\frac{\Delta t}{2}\psi_{k,t} + \frac{\Delta t^2}{4}\psi_{k,tt} + \cdots\right). \tag{3.25}$$

Note that in the expansion (3.25), the term $\frac{1}{2}\Delta t\left(\psi_{tt} + \alpha\psi_{xxt} + S\psi_t\right)$ is the derivative of the term $(\psi_t + \alpha\psi_{xx} + S\psi)$ with respect to t. Therefore, it remains

$$LTE = \left(\frac{\psi_{k,ttt}}{6} + \frac{\psi_{k,xxtt}}{2} + \frac{\overline{S}\psi_{k,tt}}{4}\right)\Delta t^2 + \alpha\left(\frac{\psi_{k,xxxx}}{12}\right)\Delta x^2 + \cdots \tag{3.26}$$

This shows the second order accuracy $O((\Delta t)^2) + O((\Delta x)^2)$ both in time and space. The method is consistent since principal part of the local truncation error goes to zero as Δx and Δt go to zero. This completes the proof. □

Now, we discuss the stability of the AVF method (3.11) by using the von Neumann stability analysis. This method is only applicable for linear system. For this reason we will consider the linear system (3.19).

Theorem 3.1.2 *The AVF method (3.11) is unconditionally stable and convergent in linear sense.*

Proof. According to the von Neumann stability analysis, we assume that

$$\psi_{1}{}_j^n = a\xi_1^n e^{i\beta j\Delta x}, \tag{3.27}$$

where $a \in \mathbb{R}$ and $\xi_1 \in \mathbb{R}$ is the amplification factor. If we substitute (3.27) into the first equation of (3.20) we get

$$i(\xi_1 - 1) + r\left(\xi_1 e^{-i\beta\Delta x} - 2\xi_1 + \xi_1 e^{i\beta\Delta x} + e^{-i\beta\Delta x} - 2 + e^{i\beta\Delta x}\right) + \frac{\overline{S}_1\Delta t}{2}(\xi_1 + 1) = 0,$$

or

$$
\begin{aligned}
i(\xi_1 - 1) &= -r\xi_1\left(e^{-i\beta\Delta x} + e^{i\beta\Delta x} - 2\right) + r\left(e^{-i\beta\Delta x} + e^{i\beta\Delta x} - 2\right) - \frac{\overline{S}_1\Delta t}{2}(\xi_1 + 1) \\
&= -r(\xi_1 + 1)\left(e^{-i\beta\Delta x} + e^{i\beta\Delta x} - 2\right) - \frac{\overline{S}_1\Delta t}{2}(\xi_1 + 1) \\
&= -r(\xi_1 + 1)\left(-2\sin^2\beta\Delta x\right) - \frac{\overline{S}_1\Delta t}{2}(\xi_1 + 1) \\
&= (\xi_1 + 1)\left(2r\sin^2\beta\Delta x + \frac{\overline{S}_1 r\Delta t}{2}\right).
\end{aligned}
$$

Then,

$$
\xi_1\left(i - 2r\sin^2\beta\Delta x - \frac{\overline{S}_1 r\Delta t}{2}\right) = i + 2r\sin^2\beta\Delta x + \frac{\overline{S}_1 r\Delta t}{2}
$$

or

$$
\xi_1 = \frac{i + 2r\sin^2\beta\Delta x + \frac{\overline{S}_1 r\Delta t}{2}}{i - 2r\sin^2\beta\Delta x - \frac{\overline{S}_1 r\Delta t}{2}}
$$

where $r = \dfrac{\alpha\Delta t}{\Delta x^2}$. Adopting the same procedure to the other equations in (3.19), we get

$$
\xi_2 = \frac{i + 2r\sin^2\beta\Delta x + \frac{\overline{S}_2 r\Delta t}{2}}{i - 2r\sin^2\beta\Delta x - \frac{\overline{S}_2 r\Delta t}{2}},
$$

$$
\xi_3 = \frac{i + 2r\sin^2\beta\Delta x + \frac{\overline{S}_1 r\Delta t}{2}}{i - 2r\sin^2\beta\Delta x - \frac{\overline{S}_1 r\Delta t}{2}}.
$$

Therefore

$$
|\xi_1| = 1, \qquad |\xi_2| = 1, \qquad |\xi_3| = 1,
$$

which shows that the AVF method is unconditionally stable in the linear sense. According to the Lax theorem the method is convergent since it is consistent and unconditionally stable [54]. □

3.2 A Linearly Implicit Scheme for 3-CNLS equation

In the previous section we have seen that the AVF scheme (3.11) is fully nonlinear which requires nonlinear solver such as Newton's iteration. In Newton's iteration, we must calculate the Jacobian matrix (3.16) in each time interval $[t_n, t_{n+1}]$, which is time consuming. The objective of this section is to develop and analyze a linearly implicit numerical method for the solution of 3–CNLS equation (2.2).

We consider the 3-CNLS equation (2.2) with initial conditions (2.3)

$$
\psi_k(x, 0) = \psi_{k,0}(x), \quad k = 1, 2, 3
$$

and periodic boundary conditions (2.4)

$$\psi_k(x_L, t) = \psi_k(x_R, t), \quad k = 1, 2, 3.$$

Following [46, 57], we propose the linearly implicit two–step (or three levels) scheme for the numerical solution of 3 − −CNLS equation (2.2),

$$\begin{aligned}
i\frac{\psi_{1,j}^{n+1} - \psi_{1,j}^{n-1}}{2\Delta t} &+ \alpha_1\delta_x^2\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^{n-1}}{2}\right) + (S_1)_j^n\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^{n-1}}{2}\right) = 0,\\
i\frac{\psi_{2,j}^{n+1} - \psi_{2,j}^{n-1}}{2\Delta t} &+ \alpha_2\delta_x^2\left(\frac{\psi_{2,j}^{n+1} + \psi_{2,j}^{n-1}}{2}\right) + (S_2)_j^n\left(\frac{\psi_{2,j}^{n+1} + \psi_{2,j}^{n-1}}{2}\right) = 0,\\
i\frac{\psi_{3,j}^{n+1} - \psi_{3,j}^{n-1}}{2\Delta t} &+ \alpha_3\delta_x^2\left(\frac{\psi_{3,j}^{n+1} + \psi_{3,j}^{n-1}}{2}\right) + (S_1)_j^n\left(\frac{\psi_{3,j}^{n+1} + \psi_{3,j}^{n-1}}{2}\right) = 0,
\end{aligned} \tag{3.28}$$

where

$$\delta_x^2\psi_j^n = \frac{1}{\Delta x^2}\left(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n\right),$$

$$(S_1)_j^n = \sigma|\psi_{1,j}^n|^2 + e|\psi_{2,j}^n|^2 + \sigma|\psi_{3,j}^n|^2, \quad (S_2)_j^n = e|\psi_{1,j}^n|^2 + \sigma|\psi_{2,j}^n|^2 + e|\psi_{3,j}^n|^2.$$

This method is of second order in time and space. It is a linearly implicit two–step method which is not self-starting. In order to start the iteration in (3.28), two initial values ψ_j^0 and ψ_j^1 are required. ψ^0 is obtained from the initial condition. ψ^1 can be obtained from the Forward Euler method with a small step size $\Delta t = 0.0001$. Then, $\psi^2, \psi^3, \cdots$ are obtained from the two-step scheme (3.28).

Theorem 3.2.1 *The two-step scheme (3.28) is conservative in the sense that*

$$\begin{aligned}
Q_1^n &= \sum_{j=1}^{N}\left(|\psi_{1}{}_j^{n+1}|^2 + |\psi_{1}{}_j^{n}|^2\right) = Q_1^{n-1} = \cdots = Q_1^0,\\
Q_2^n &= \sum_{j=1}^{N}\left(|\psi_{2}{}_j^{n+1}|^2 + |\psi_{2}{}_j^{n}|^2\right) = Q_2^{n-1} = \cdots = Q_2^0,\\
Q_3^n &= \sum_{j=1}^{N}\left(|\psi_{3}{}_j^{n+1}|^2 + |\psi_{3}{}_j^{n}|^2\right) = Q_3^{n-1} = \cdots = Q_3^0,
\end{aligned} \tag{3.29}$$

for $n = 0, 1, 2, \cdots, N$, *where* Q_1^n, Q_2^n *and* Q_3^n *are discrete masses.*

Proof. In order to show that the proposed scheme (3.28) has conserved quantity Q_1^n, we multiply the the first equation in (3.28) by $(\overline{\psi_{1,j}^{n+1}} + \overline{\psi_{1,j}^{n-1}})$, which gives

$$i\left(\overline{\psi_{1,j}^{n+1}} + \overline{\psi_{1,j}^{n-1}}\right)\left(\frac{\psi_{1,j}^{n+1} - \psi_{1,j}^{n-1}}{2\Delta t}\right) + \alpha_1\left(\overline{\psi_{1,j}^{n+1}} + \overline{\psi_{1,j}^{n-1}}\right)\delta_x^2\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^{n-1}}{2}\right) + (S_1)_j^n\left(\overline{\psi_{1,j}^{n+1}} + \overline{\psi_{1,j}^{n-1}}\right)\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^{n-1}}{2}\right) = 0. \tag{3.30}$$

The first term in the multiplication (3.30) gives

$$
\begin{aligned}
i\left(\overline{\psi_{1,j}^{n+1}}+\overline{\psi_{1,j}^{n-1}}\right)\left(\frac{\psi_{1,j}^{n+1}-\psi_{1,j}^{n-1}}{2\Delta t}\right) &= \frac{i}{2\Delta t}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}-\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n-1}}\right) \\
&= \frac{i}{2\Delta t}\left\{\left(\left|\psi_{1,j}^{n+1}\right|^2-\left|\psi_{1,j}^{n-1}\right|^2\right)+\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}-\overline{\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}}\right\} \\
&= \frac{i}{2\Delta t}\left(\left|\psi_{1,j}^{n+1}\right|^2-\left|\psi_{1,j}^{n-1}\right|^2\right)+\text{ real terms.} \qquad (3.31)
\end{aligned}
$$

The second term in the multiplication (3.30) gives

$$
\begin{aligned}
&\alpha_1\left(\overline{\psi_{1,j}^{n+1}}+\overline{\psi_{1,j}^{n-1}}\right)\delta_x^2\left(\frac{\psi_{1,j}^{n+1}+\psi_{1,j}^{n-1}}{2}\right) \\
&= \frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j-1}^{n+1}-2\psi_{1,j}^{n+1}+\psi_{1,j+1}^{n+1}+\psi_{1,j-1}^{n-1}-2\psi_{1,j}^{n-1}+\psi_{1,j+1}^{n-1}\right)\left(\overline{\psi_{1,j}^{n+1}}+\overline{\psi_{1,j}^{n-1}}\right) \\
&= \frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j-1}^{n+1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j-1}^{n+1}\overline{\psi_{1,j}^{n-1}}+\psi_{1,j-1}^{n-1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j-1}^{n-1}\overline{\psi_{1,j}^{n-1}}\right) \qquad (3.32) \\
&+ \frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n-1}}+\psi_{1,j+1}^{n-1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j+1}^{n-1}\overline{\psi_{1,j}^{n-1}}\right) \qquad (3.33) \\
&+ \frac{\alpha_1}{2\Delta x^2}\left(-2\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}}-2\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}-2\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n+1}}-2\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n-1}}\right). \qquad (3.34)
\end{aligned}
$$

Shifting the index $j-1$ to j and taking the sum (3.32) over j yields,

$$
\begin{aligned}
&\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,i+1}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,i+1}^{n-1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,i+1}^{n+1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,i+1}^{n-1}}\right) \\
&+\left(\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n+1}}+\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n-1}}+\psi_{1,0}^{n-1}\overline{\psi_{1,1}^{n+1}}+\psi_{1,0}^{n-1}\overline{\psi_{1,1}^{n-1}}\right) \\
&+\left(\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n+1}}+\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n-1}}+\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n+1}}+\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n-1}}\right) \\
&-\left(\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n+1}}+\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n-1}}+\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n+1}}+\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n-1}}\right) \\
&=\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,i+1}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,i+1}^{n-1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,i+1}^{n+1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,i+1}^{n-1}}\right) \\
&+\left(\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n+1}}+\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n-1}}+\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n+1}}+\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n-1}}\right) \\
&-\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n+1}}-\psi_{1,J}^{n+1}\overline{\psi_{1,J+1}^{n-1}}-\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n+1}}-\psi_{1,J}^{n-1}\overline{\psi_{1,J+1}^{n-1}}+\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n+1}}+\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n-1}}+\psi_{1,0}^{n-1}\overline{\psi_{1,1}^{n+1}}+\psi_{1,0}^{n-1}\overline{\psi_{1,1}^{n-1}}
\end{aligned}
$$

By using the periodic boundary conditions $\psi_J^{n+1}=\psi_0^{n+1}$ and $\psi_J^{n-1}=\psi_0^{n-1}$ and taking sum over j again, we get

$$
\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n-1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,j+1}^{n+1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,j+1}^{n-1}}\right). \qquad (3.35)
$$

Applying the same procedure to the equations (3.33), (3.34), the equations (3.32), (3.33) and (3.34) simplified to

$$\frac{\alpha_1}{2\Delta x^2}\left\{\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n+1}}\right)+\left(\psi_{1,j+1}^{n-1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n-1}}\right)\right.$$
$$+\left(\psi_{1,j+1}^{n-1}\overline{\psi_{1,j}^{n-1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,j+1}^{n-1}}\right)+\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n-1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,j+1}^{n+1}}\right)$$
$$-2\left|\psi_{1,j}^{n+1}\right|^2-2\left|\psi_{1,j}^{n-1}\right|^2-2\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}+\overline{\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}}\right) \tag{3.36}$$

which is real since

$$(a+ib)\overline{(c+id)}+\overline{(a+ib)}(c+id)=2(ac+bd)$$

is real. Finally, the nonlinear term in the multiplication (3.30) gives

$$(S_1)_j^n\left(\overline{\psi_{1,j}^{n+1}}+\overline{\psi_{1,j}^{n-1}}\right)\left(\frac{\psi_{1,j}^{n+1}+\psi_{1,j}^{n-1}}{2}\right)$$
$$=(S_1)_j^n\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n-1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n-1}}\right)$$
$$=\left|\psi_{1,j}^{n+1}\right|^2+\left|\psi_{1,j}^{n-1}\right|^2+\left(\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n+1}}+\overline{\psi_{1,j}^{n-1}\overline{\psi_{1,j}^{n+1}}}\right), \tag{3.37}$$

which is real, too. Thus, multiplying the first equation in (3.28) by $(\overline{\psi_{1,j}^{n+1}}+\overline{\psi_{1,j}^{n-1}})$, summing over j and taking the imaginary terms in the multiplication yields

$$\sum_{j=1}^{J}\left(\left|\psi_{1,j}^{n+1}\right|^2-\left|\psi_{1,j}^{n-1}\right|^2\right)=0$$

or

$$\sum_{j=1}^{J}\left(\left|\psi_{1,j}^{n+1}\right|^2+\left|\psi_{1,j}^{n}\right|^2\right)=\sum_{j=1}^{J}\left(\left|\psi_{1,j}^{n}\right|^2+\left|\psi_{1,j}^{n-1}\right|^2\right).$$

This means that

$$Q_1^n=Q_1^{n-1}\ldots=Q_1^0$$

and it completes the proof of the first charge conservation law in (3.29). Second and third conservations in (3.29) can be proven similarly. □

3.2.1 Linear Stability Analysis

In this section, we will explore the accuracy, stability and truncation error of the two–step scheme (3.28). The notion of accuracy and consistency is crucial to understand how well a numerical scheme approximates an equation. We first discuss the accuracy of the scheme (3.28).

Theorem 3.2.2 *The two step method (3.28) for* 3*-CNLSE is a consistent method with the accuracy of* $\mathcal{O}((\Delta t)^2)+\mathcal{O}((\Delta x)^2)$.

Proof. We start by assuming that the numerical method (3.28) is exact at the grid point (x_j, t_n). Then the local truncation error is

$$T(x_j,t_n) := \frac{\psi_k(x_j,t_{n+1})-\psi_k(x_j,t_{n-1})}{2\Delta t} + \alpha_k\delta_x^2\left(\frac{\psi_k(x_j,t_{n+1})+\psi_k(x_j,t_{n-1})}{2}\right) + (\overline{S})_j^n\left(\frac{\psi_k(x_j,t_{n+1})+\psi_k(x_j,t_{n-1})}{2}\right), \quad k=1,2,3, \quad (3.38)$$

where $\overline{S} = S_1$ for $k = 1,3$ and $\overline{S} = S_2$ for $k = 2$. By using Taylor Series expansion about (x_j, t_n), we obtain the followings:

The first term of (3.38):

$$\frac{\psi_k(x_j,t_{n+1})-\psi_k(x_j,t_{n-1})}{2\Delta t} = \left(2\Delta t\psi_{k,t} + \frac{\Delta t^3}{6}\psi_{k,ttt} + ...\right); \quad (3.39)$$

The second term of (3.38):

$$\frac{\alpha_k}{2}\left(\frac{\psi_k(x_{j-1},t_{n+1})-2\psi_k(x_j,t_{n+1})+\psi_k(x_{j+1},t_{n+1})}{\Delta x^2} + \frac{\psi_k(x_{j-1},t_{n-1})-2\psi_k(x_j,t_{n-1})+\psi_k(x_{j+1},t_{n-1})}{\Delta x^2}\right)$$
$$= \frac{\alpha_k}{2\Delta x^2}\left(4\psi_{k,xx}\frac{\Delta x^2}{2} + 4\psi_{k,xxxx}\frac{\Delta x^4}{24} + 6\psi_{k,xxtt}\frac{\Delta x^2\Delta t^2}{4} + ...\right); \quad (3.40)$$

The third term of (3.38):

$$(\overline{S})_j^n\frac{\psi_k(x_j,t_{n+1})+\psi_k(x_j,t_{n-1})}{2} = \frac{(\overline{S})_j^n}{2}\left(2\psi_k + \Delta t^2\psi_{k,tt} + ...\right), \quad (3.41)$$

where each term on the right hand side is evaluated at (x_j, t_n). Summing up (3.39), (3.40) and (3.41) yields the truncation error

$$LTE \;=\; \left(\psi_{k,t} + \alpha_1\psi_{k,xx} + (\overline{S})_j^n\psi_k\right) \;+\; \left(\frac{\Delta t^2}{6}\psi_{k,ttt} + \frac{\Delta x^2}{12}\psi_{k,xxxx} + \frac{\Delta t^2}{4}\psi_{k,xxtt} + \frac{\Delta t^2}{2}(\overline{S})_j^n\psi_{k,tt}\right) \quad (3.42)$$

or

$$LTE = \left(\frac{\psi_{k,ttt}}{6} + \frac{1}{4}\psi_{k,xxtt}\right)\Delta t^2 + \left(\frac{1}{12}\psi_{k,xxxx} + \frac{1}{2}(\overline{S})_j^n\psi_{k,tt}\right)\Delta x^2 + O(\Delta t^3) + O(\Delta x^3), \quad (3.43)$$

which shows that the two–step method (3.28) has the accuracy of $O((\Delta t)^2) + O((\Delta x)^2)$.

Note that the two–step scheme (3.28) is consistent with the 3−CNLS equation (2.2), since

$$\left(\frac{\psi_{k,ttt}}{6} + \frac{1}{4}\psi_{k,xxtt}\right)\Delta t^2 + \left(\frac{1}{12}\psi_{k,xxxx} + \frac{1}{2}(\overline{S})_j^n\psi_{k,tt}\right)\Delta x^2 \to 0$$

as $(\Delta t, \Delta x) \to (0,0)$. This completes the proof. □

Theorem 3.2.3 *The two step method (3.28) is unconditionally stable in linear sense.*

Proof. Application of the two–step scheme (3.28) to the linear 3−CNLS equation (3.19) yields

$$\begin{aligned} i\frac{{\psi_1}_j^{n+1}-{\psi_1}_j^{n-1}}{2\Delta t} + \alpha_1\delta_x^2\left(\frac{{\psi_1}_j^{n+1}+{\psi_1}_j^{n-1}}{2\Delta x^2}\right) + \overline{S_1}\frac{{\psi_1}_j^{n+1}+{\psi_1}_j^{n-1}}{2} &= 0, \\ i\frac{{\psi_2}_j^{n+1}-{\psi_2}_j^{n-1}}{2\Delta t} + \alpha_2\delta_x^2\left(\frac{{\psi_2}_j^{n+1}+{\psi_2}_j^{n-1}}{2\Delta x^2}\right) + \overline{S_2}\frac{{\psi_2}_j^{n+1}+{\psi_2}_j^{n-1}}{2} &= 0, \\ i\frac{{\psi_3}_j^{n+1}-{\psi_3}_j^{n-1}}{2\Delta t} + \alpha_3\delta_x^2\left(\frac{{\psi_3}_j^{n+1}+{\psi_3}_j^{n-1}}{2\Delta x^2}\right) + \overline{S_1}\frac{{\psi_3}_j^{n+1}+{\psi_3}_j^{n-1}}{2} &= 0, \end{aligned} \tag{3.44}$$

where $\overline{S_1}$ and $\overline{S_2}$ are constants (see [57])

$$\begin{aligned} \overline{S_1} &= \max_{j=1,\cdots,M}\{\sigma|\psi_1^n| + e|\psi_2^n| + \sigma|\psi_3^n|\}, \\ \overline{S_2} &= \max_{j=1,\cdots,M}\{e|\psi_1^n| + \sigma|\psi_2^n| + e|\psi_3^n|\}. \end{aligned} \tag{3.45}$$

Consider the first equation in (3.44). By using the von Neumann stability analysis we set

$${\psi_1}_j^n = \xi_1^n e^{i\beta j\Delta x}, \quad {\psi_1}_j^{n+1} = \xi_1^n \xi e^{i\beta\ j\Delta x}, \quad {\psi_1}_j^{n-1} = \xi_1^n \xi_1^{-1} e^{i\beta j\Delta x},$$

where $\beta \in \mathbb{R}$ and $\xi_1 \in \mathbb{R}$ is the amplification factor. If we substitute these into the first equation of (3.44), we get

$$i\left(\xi_1 - \xi_1^{-1}\right) + r\left(\xi_1\left(e^{i\beta\Delta x} + e^{-i\beta\Delta x}\right) + \xi_1^{-1}\left(e^{i\beta\Delta x} + e^{-i\beta\Delta x}\right) - 2\left(\xi_1 + \xi_1^{-1}\right)\right) + \frac{\bar{S_1}\Delta t}{2}\left(\xi_1 + \xi_1^{-1}\right) = 0$$

or

$$i\left(\xi_1 - \xi_1^{-1}\right) + r\left(\left(e^{i\beta\Delta x} + e^{-i\beta\Delta x} - 2\right)\left(\xi_1 + \xi_1^{-1}\right)\right) + \frac{\bar{S_1}\Delta t}{2}\left(\xi_1 + \xi_1^{-1}\right) = 0.$$

Solving this equation for ξ_1

$$\begin{aligned} i\left(\xi_1 - \xi_1^{-1}\right) &= -\left(\xi_1 + \xi_1^{-1}\right)\left(r(2\cos\beta\Delta x - 2) + \frac{\bar{S_1}\Delta t}{2}\right), \\ i\left(\frac{\xi_1 - \xi_1^{-1}}{\xi_1 + \xi_1^{-1}}\right) &= r(2 - 4\sin^2\frac{\beta\Delta x}{2} - 2) + \frac{\bar{S_1}\Delta t}{2}, \\ \xi_1(i + 4r\sin^2\frac{\beta\Delta x}{2} - \frac{\bar{S}\Delta t}{2}) &= \xi_1^{-1}(i - 4r\sin^2\frac{\beta\Delta x}{2} + \frac{\bar{S_1}\Delta t}{2}) \end{aligned}$$

and therefore

$$\xi_1^2 = \frac{i - 4r\sin^2\frac{\beta\Delta x}{2} + \frac{\bar{S_1}\Delta t}{2}}{i + 4r\sin^2\frac{\beta\Delta x}{2} - \frac{\bar{S_1}\Delta t}{2}}.$$

Then taking the norm of both sides one gets

$$|\xi_1|^2 = \left|\frac{i - (4r\sin^2\frac{\beta\Delta x}{2} - \frac{\bar{S_1}\Delta t}{2})}{i + 4r\sin^2\frac{\beta\Delta x}{2} - \frac{\bar{S_1}\Delta t}{2}}\right|,$$

which means that

$$|\xi_1|^2 = 1 \Rightarrow |\xi_1| = 1,$$

where $r = \frac{\alpha_k\Delta t}{\Delta x^2}, k = 1, 2, 3$. Applying the same procedure for the second and third equations in (3.44) it can be shown that

$$|\xi_2| = 1 \qquad \text{and} \qquad |\xi_3| = 1,$$

which shows that the two step scheme is unconditionally stable in the linear sense. □

According to the Lax theorem the method is convergent since it is consistent and unconditionally stable [54].

3.3 A One–step Scheme for 3–CNLS Equation

In sections Sec. 3.1 and Sec. 3.2 we have proposed two methods for the numerical solution of the 3–CNLS equation (2.2). The scheme (3.11) introduced in Sec. 3.1 was energy conserving but not mass conserving while the scheme (3.28) introduced in Sec. 3.2 was mass conserving but not energy conserving. The objective of this section is to introduce and analyze a numerical method for the 3–CNLS equation (2.2) which is both energy conserving and mass conserving.

In this section, we consider the 3-CNLS equation (2.2) with the initial conditions (2.3)

$$\psi_k(x,0) = \psi_{k0}(x), \quad k = 1,2,3$$

and the homogenous boundary conditions (2.5)

$$\psi_k(x_L,t) = \psi_k(x_R,t) = 0, \quad k = 1,2,3.$$

Let z_j^n be an approximation to $z\left(x_j,t_n\right)$ and w_j^n be an approximation to $w\left(x_j,t_n\right)$. We introduce the following notations:

$$\begin{aligned}
&\langle z^n, w^n\rangle = h\sum_{j=1}^{M-1} z_j^n\overline{w_j^n}, && \|w^n\|^2 = \langle w^n, w^n\rangle\,,\\
&\|(w^n)_x\|^2 = h\sum_{j=1}^{M-1}\left|\left(w_j^n\right)_x\right|^2, && \|w^n\|^4 = h\sum_{j=1}^{M-1}\left|w_j^n\right|^4,\\
&\|w^n\|_\infty = \max_{1\le j\le M}\left|w_j^n\right|, && \delta_x^2 z_j^n = \frac{z_{j-1}^n - 2z_j^n + z_{j+1}^n}{\Delta x^2}.
\end{aligned} \tag{3.46}$$

Following [49], we introduced the one–step (or two levels) finite difference scheme for the 3−CNLS equation (2.2)

$$\begin{aligned}
i\frac{\psi_{1,j}^{n+1} - \psi_{1,j}^n}{\Delta t} &+ \alpha_1\delta_x^2\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^n}{2}\right) + S_{1,j}^{\,n}\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^n}{2}\right) = 0,\\
i\frac{\psi_{2,j}^{n+1} - \psi_{2,j}^n}{2\Delta t} &+ \alpha_2\delta_x^2\left(\frac{\psi_{2,j}^{n+1} + \psi_{2,j}^n}{2}\right) + S_{2,j}^{\,n}\left(\frac{\psi_{2,j}^{n+1} + \psi_{2,j}^n}{2}\right) = 0,\\
i\frac{\psi_{3,j}^{n+1} - \psi_{3,j}^n}{2\Delta t} &+ \alpha_3\delta_x^2\left(\frac{\psi_{3,j}^{n+1} + \psi_{3,j}^n}{2}\right) + S_{1,j}^{\,n}\left(\frac{\psi_{3,j}^{n+1} + \psi_{3,j}^n}{2}\right) = 0,
\end{aligned} \tag{3.47}$$

where

$$S_{1,j}^{\,n} = \frac{1}{2}\left[\sigma\left(\left|\psi_{1,j}^{n+1}\right|^2 + \left|\psi_{1,j}^n\right|^2\right) + e\left(\left|\psi_{2,j}^{n+1}\right|^2 + \left|\psi_{2,j}^n\right|^2\right) + \sigma\left(\left|\psi_{3,j}^{n+1}\right|^2 + \left|\psi_{3,j}^n\right|^2\right)\right],$$

$$S^{n}_{2,j} = \frac{1}{2}\left[\, e\left(\left|\psi^{n+1}_{1,j}\right|^2 + \left|\psi^{n}_{1,j}\right|^2\right) + \sigma\left(\left|\psi^{n+1}_{2,j}\right|^2 + \left|\psi^{n}_{2,j}\right|^2\right) + \; e\left(\left|\psi^{n+1}_{3,j}\right|^2 + \left|\psi^{n}_{3,j}\right|^2\right)\right].$$

Note that the scheme (3.47) is the Crank–Nicolson scheme for the equation (2.2). Since more than one unknowns are involved for each j in the equation (3.47), the scheme (3.47) is an implicit scheme. For linear equations, the Crank–Nicolson scheme produce sparse linear algebraic equations, since the finite difference equation at any time level t_{n+1} has only three unknown coefficients involving space nodes $j-1$, j, and $j+1$. In matrix notation these equations can be written as $Ax = b$. However, the system of discrete equations (3.47) is nonlinear, therefore, one has to solve a system of non-linear algebraic equations for every time interval $t_n \le t \le t_{n+1}$.

The equations (3.47) yield $6M$ nonlinear systems of equations

$$\begin{aligned} F_{1,j} = \left(a^{n+1}_j - a^n_j\right) - \frac{\alpha_1 \Delta t}{2\Delta x^2}\left(b^n_{j-1} - 2b^n_j + b^n_{j+1} + b^{n+1}_{j-1} - 2b^{n+1}_j + b^{n+1}_{j+1}\right) \\ - \frac{\Delta t}{2}\Big\{\sigma\left[(a^n_j)^2 + (a^{n+1}_j)^2 + (b^n_j)^2 + (b^{n+1}_j)^2\right] \\ + e\left[(p^n_j)^2 + (p^{n+1}_j)^2 + (q^n_j)^2 + (q^{n+1}_j)^2\right] \\ +\sigma\left[(u^n_j)^2 + (u^{n+1}_j)^2 + (v^n_j)^2 + (v^{n+1}_j)^2\right]\Big\}\frac{b^n_j + b^{n+1}_j}{2} d\xi, \end{aligned}$$

$$\begin{aligned} F_{2,j} = \left(p^{n+1}_j - p^n_j\right) - \frac{\alpha_2 \Delta t}{2\Delta x^2}\left(q^n_{j-1} - 2q^n_j + b^n_{j+1} + q^{n+1}_{j-1} - 2q^{n+1}_j + q^{n+1}_{j+1}\right) \\ - \frac{\Delta t}{2}\Big\{e\left[(a^n_j)^2 + (a^{n+1}_j)^2 + (b^n_j)^2 + (b^{n+1}_j)^2\right] \\ + \sigma\left[(p^n_j)^2 + (p^{n+1}_j)^2 + (q^n_j)^2 + (q^{n+1}_j)^2\right] \\ +e\left[(u^n_j)^2 + (u^{n+1}_j)^2 + (v^n_j)^2 + (v^{n+1}_j)^2\right]\Big\}\frac{q^n_j + q^{n+1}_j}{2} d\xi, \end{aligned}$$

$$\begin{aligned} F_{3,j} = \left(u^{n+1}_j - u^n_j\right) - \frac{\alpha_3 \Delta t}{2\Delta x^2}\left(v^n_{j-1} - 2v^n_j + v^n_{j+1} + v^{n+1}_{j-1} - 2v^{n+1}_j + v^{n+1}_{j+1}\right) \\ - \frac{\Delta t}{2}\Big\{\sigma\left[(a^n_j)^2 + (a^{n+1}_j)^2 + (b^n_j)^2 + (b^{n+1}_j)^2\right] \\ + e\left[(p^n_j)^2 + (p^{n+1}_j)^2 + \left(q^n_j\right)^2 + (q^{n+1}_j)^2\right] \\ +\sigma\left[(u^n_j)^2 + (u^{n+1}_j)^2 + (v^n_j)^2 + (v^{n+1}_j)^2\right]\Big\}\frac{v^n_j + v^{n+1}_j}{2} d\xi, \end{aligned}$$

$$F_{4,j} = \left(b_j^{n+1} - b_j^n\right) + \frac{\alpha_1 \Delta t}{2\Delta x^2}\left(a_{j-1}^n - 2a_j^n + a_{j+1}^n + a_{j-1}^{n+1} - 2a_j^{n+1} + a_{j+1}^{n+1}\right)$$
$$+ \frac{\Delta t}{2}\left\{\sigma\left[(a_j^n)^2 + (a_j^{n+1})^2 + (b_j^n)^2 + (b_j^{n+1})^2\right]\right.$$
$$+ e\left[(p_j^n)^2 + (p_j^{n+1})^2 + (q_j^n)^2 + (q_j^{n+1})^2\right]$$
$$\left.+\sigma\left[(u_j^n)^2 + (u_j^{n+1})^2 + (v_j^n)^2 + (v_j^{n+1})^2\right]\right\}\frac{a_j^n + a_j^{n+1}}{2} d\xi,$$

$$F_{5,j} = \left(q_j^{n+1} - q_j^n\right) + \frac{\alpha_2 \Delta t}{2\Delta x^2}\left(p_{j-1}^n - 2p_j^n + p_{j+1}^n + p_{j-1}^{n+1} - 2p_j^{n+1} + p_{j+1}^{n+1}\right)$$
$$+ \frac{\Delta t}{2}\left\{ e\left[(a_j^n)^2 + (a_j^{n+1})^2 + (b_j^n)^2 + (b_j^{n+1})^2\right]\right.$$
$$+ \sigma\left[(p_j^n)^2 + (p_j^{n+1})^2 + (q_j^n)^2 + (q_j^{n+1})^2\right]$$
$$\left.+e\left[(u_j^n)^2 + (u_j^{n+1})^2 + (v_j^n)^2 + (v_j^{n+1})^2\right]\right\}\frac{p_j^n + p_j^{n+1}}{2} d\xi$$

and

$$F_{6,j} = \left(v_j^{n+1} - v_j^n\right) + \frac{\alpha_3 \Delta t}{2\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n + u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}\right)$$
$$+ \frac{\Delta t}{2}\left\{\sigma\left[(a_j^n)^2 + (a_j^{n+1})^2 + (b_j^n)^2 + (b_j^{n+1})^2\right]\right.$$
$$+ e\left[(p_j^n)^2 + (p_j^{n+1})^2 + (q_j^n)^2 + (q_j^{n+1})^2\right]$$
$$\left.+\sigma\left[(u_j^n)^2 + (u_j^{n+1})^2 + (v_j^n)^2 + (v_j^{n+1})^2\right]\right\}\frac{u_j^n + u_j^{n+1}}{2} d\xi,$$

with the Jacobian matrix J

$$J = \begin{bmatrix}
\frac{\partial F_{1,j}}{\partial a_j^{n+1}} & \frac{\partial F_{1,j}}{\partial b_j^{n+1}} & \frac{\partial F_{1,j}}{\partial p_j^{n+1}} & \frac{\partial F_{1,j}}{\partial q_j^{n+1}} & \frac{\partial F_{1,j}}{\partial u_j^{n+1}} & \frac{\partial F_{1,j}}{\partial v_j^{n+1}} \\
\frac{\partial F_{2,j}}{\partial a_j^{n+1}} & \frac{\partial F_{2,j}}{\partial b_j^{n+1}} & \frac{\partial F_{2,j}}{\partial p_j^{n+1}} & \frac{\partial F_{2,j}}{\partial q_j^{n+1}} & \frac{\partial F_{2,j}}{\partial u_j^{n+1}} & \frac{\partial F_{2,j}}{\partial v_j^{n+1}} \\
\frac{\partial F_{3,j}}{\partial a_j^{n+1}} & \frac{\partial F_{3,j}}{\partial b_j^{n+1}} & \frac{\partial F_{3,j}}{\partial p_j^{n+1}} & \frac{\partial F_{3,j}}{\partial q_j^{n+1}} & \frac{\partial F_{3,j}}{\partial u_j^{n+1}} & \frac{\partial F_{3,j}}{\partial v_j^{n+1}} \\
\frac{\partial F_{4,j}}{\partial a_j^{n+1}} & \frac{\partial F_{4,j}}{\partial b_j^{n+1}} & \frac{\partial F_{4,j}}{\partial p_j^{n+1}} & \frac{\partial F_{4,j}}{\partial q_j^{n+1}} & \frac{\partial F_{4,j}}{\partial u_j^{n+1}} & \frac{\partial F_{4,j}}{\partial v_j^{n+1}} \\
\frac{\partial F_{5,j}}{\partial a_j^{n+1}} & \frac{\partial F_{5,j}}{\partial b_j^{n+1}} & \frac{\partial F_{5,j}}{\partial p_j^{n+1}} & \frac{\partial F_{5,j}}{\partial q_j^{n+1}} & \frac{\partial F_{5,j}}{\partial u_j^{n+1}} & \frac{\partial F_{5,j}}{\partial v_j^{n+1}} \\
\frac{\partial F_{6,j}}{\partial a_j^{n+1}} & \frac{\partial F_{6,j}}{\partial b_j^{n+1}} & \frac{\partial F_{6,j}}{\partial p_j^{n+1}} & \frac{\partial F_{6,j}}{\partial q_j^{n+1}} & \frac{\partial F_{6,j}}{\partial u_j^{n+1}} & \frac{\partial F_{6,j}}{\partial v_j^{n+1}}
\end{bmatrix}_{6Mx6M}. \quad (3.48)$$

Then we apply the Newton method as described in Sec. (3.1). In Newton method, three iterations satisfy

$$|\mathbf{Z}^{n+1} - \mathbf{Z}^n| < tol$$

for $tol = 10^{-7}$. When we decrease the tolerance to $tol = 10^{-15}$, four iterations satisfy the required accuracy.

Theorem 3.3.1 *The scheme (3.47) conserves the mass/charge in the sense*

$$\begin{aligned} Q_1^n &= \left\|\psi_1^n\right\|^2 = Q_1^{n-1} = \ldots = Q_1^0, \\ Q_2^n &= \left\|\psi_2^n\right\|^2 = Q_2^{n-1} = \ldots = Q_2^0, \\ Q_3^n &= \left\|\psi_3^n\right\|^2 = Q_3^{n-1} = \ldots = Q_3^0. \end{aligned} \tag{3.49}$$

Proof. We will prove the first conserved quantity

$$Q_1^n = \left\|\psi_1^n\right\|^2 = Q_1^{n-1} = \ldots = Q_1^0$$

in (3.49). Conservations of $Q_2^n = Q_2^0$ and $Q_3^n = Q_3^0$ can be shown similarly.

Multiplying the first equation in (3.47) by $\overline{\psi_{1,j}^{n+1} + \psi_{1,j}^n}$, we get

$$\frac{i}{\Delta t}\left(\psi_{1,j}^{n+1} - \psi_j^n\right) + \frac{\alpha}{2\Delta x^2}\left(\psi_{1,j+1}^{n+1} - 2\psi_{1,j}^{n+1} + \psi_{1,j-1}^{n+1} + \psi_{1,j+1}^n - 2\psi_{1,j}^{n+1} + \psi_{1,j-1}^n\right) + \frac{S_{1,j}^n}{2}\left(\psi_{1,j}^{n+1} + \psi_{1,j}^n\right)\left(\overline{\psi_{1,j}^{n+1} + \psi_j^n}\right) = 0. \tag{3.50}$$

The first product in (3.50) gives

$$\frac{i}{\Delta t}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^{n+1}\overline{\psi_{1,j}^n} - \psi_{1,j}^n\overline{\psi_{1,j}^{n+1}} - \psi_{1,j}^n\overline{\psi_{1,j}^n}\right).$$

Taking the sum from $j = 1$ to $J - 1$ leads to

$$\begin{aligned} &\frac{i}{\Delta x\Delta t}\left(\Delta x\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}} - \psi_{1,j}^n\overline{\psi_{1,j}^n}\right)\right) + \frac{i}{\Delta x\Delta t}\left(\Delta x\sum_{j=1}^{J-1}\psi_{1,j}^{n+1}\overline{\psi_{1,j}^n} - \overline{\psi_{1,j}^{n+1}\overline{\psi_{1,j}^n}}\right) \\ &= \frac{i}{\Delta x\Delta t}\left(\left\|\psi_j^{n+1}\right\|^2 - \left\|\psi_j^n\right\|^2\right) + i\frac{i}{\Delta t}\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^n} - \overline{\psi_{1,j}^{n+1}\overline{\psi_{1,j}^n}}\right) \\ &= \frac{i}{\Delta x\Delta t}\left(\left\|\psi_j^{n+1}\right\|^2 - \left\|\psi_j^n\right\|^2\right) + \text{ real terms.} \end{aligned} \tag{3.51}$$

Now taking the sum of the second term in (3.50), one obtains

$$\begin{aligned} &\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j-1}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j-1}^{n+1}\overline{\psi_{1,j}^n} + \psi_{1,j-1}^n\overline{\psi_{1,j}^{n+1}} + \psi_{1,j-1}^n\overline{\psi_{1,j}^n}\right) \\ &+ \frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^n} + \psi_{1,j+1}^n\overline{\psi_{1,j}^{n+1}} + \psi_{1,j+1}^n\overline{\psi_{1,j}^n}\right) \\ &- \frac{\alpha_1}{\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^{n+1}\overline{\psi_{1,j}^n} + \psi_{1,j}^n\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^n\overline{\psi_{1,j}^n}\right). \end{aligned} \tag{3.52}$$

Shifting $j-1$ to j in the first term above, and using the homogenous boundary conditions $\psi_{k,0} = \psi_{k,J} = 0, k = 1,2,3.$

$$\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-2}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n+1}} + \psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n}} + \psi_{1,j}^{n}\overline{\psi_{1,j+1}^{n+1}} + \psi_{1,j}^{n}\overline{\psi_{1,j+1}^{n}}\right)$$
$$+\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n+1}} + \psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n}} + \psi_{1,0}^{n}\overline{\psi_{1,1}^{n+1}} + \psi_{1,0}^{n}\overline{\psi_{1,1}^{n}} \pm \psi_{1,J-1}^{n+1}\overline{\psi_{1,J}^{n+1}} \pm \psi_{1,J-1}^{n+1}\overline{\psi_{1,J}^{n}} \pm \psi_{1,J-1}^{n}\overline{\psi_{1,J}^{n+1}} \pm \psi_{1,J-1}^{n}\overline{\psi_{1,J}^{n}}$$
$$+\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n}} + \psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n}}\right)$$
$$-\frac{\alpha_1}{\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}} + \psi_{1,j}^{n}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^{n}\overline{\psi_{1,j}^{n}}\right), \quad (3.53)$$

we obtain

$$\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n+1}} + \psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n}} + \psi_{1,j}^{n}\overline{\psi_{1,j+1}^{n+1}} + \psi_{1,j}^{n}\overline{\psi_{1,j+1}^{n}}\right)$$
$$+\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n}} + \psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n}}\right)$$
$$-\frac{\alpha_1}{\Delta x^2}\sum_{j=1}^{J-1}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}} + \psi_{1,j}^{n}\overline{\psi_{1,j}^{n+1}} + \psi_{1,j}^{n}\overline{\psi_{1,j}^{n}}\right), \quad (3.54)$$

which is all real. The third term in (3.50)

$$\frac{S_{1,j}^{n}}{2}\left(\psi_{1,j}^{n+1} + \psi_{1,j}^{n}\right)\left(\overline{\psi_{1,j}^{n+1} + \psi_{j}^{n}}\right) = S_{1,j}^{n}\left(\left|\psi_{1,j}^{n+1}\right|^2 + \left|\psi_{1,j}^{n}\right|^2 + \psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}} + \overline{\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}}}\right) \quad (3.55)$$

is a real number, too. Taking the imaginary part of (3.50), we obtain $\left\|\psi_j^{n+1}\right\|^2 - \left\|\psi_j^{n}\right\|^2 = 0$ or

$$\left\|\psi_j^{n+1}\right\|^2 = \left\|\psi_j^{n}\right\|^2 = \left\|\psi_j^{n-1}\right\|^2 = \cdots = \left\|\psi_j^{0}\right\|^2.$$

which completes the first conserved quantity in (3.49). □

Theorem 3.3.2 *The scheme (3.47) conserves energy (2.13) in the sense*

$$E^n = \frac{-1}{2}\left(\alpha_1\left\|\psi_{1x}^n\right\|^2 + \alpha_2\left\|\psi_{2x}^n\right\|^2 + \alpha_3\left\|\psi_{3x}^n\right\|^2\right) + \frac{\sigma}{4}\left(\left\|\psi_{1,j}\right\|_4^4 + \left\|\psi_{2,j}\right\|_4^4 + \left\|\psi_{3,j}\right\|_4^4\right)$$
$$+\frac{e\Delta x}{2}\sum_{j=1}^{M-1}\left|\psi_{1,j}^n\right|^2\left|\psi_{2,j}^n\right|^2 + \frac{\sigma\Delta x}{2}\sum_{j=1}^{M-1}\left|\psi_{2,j}^n\right|^2\left|\psi_{3,j}^n\right|^2 + \frac{e\Delta x}{2}\sum_{j=1}^{M-1}\left|\psi_{1,j}^n\right|^2\left|\psi_{3,j}^n\right|^2$$
$$= E^{n-1} = \ldots = E^0. \quad (3.56)$$

Proof. We multiply the first equation of (3.47) by $\overline{\psi_{1,j}^{n+1} - \psi_{1,j}^{n}}$ and get

$$\left(i\frac{\psi_{1,j}^{n+1} - \psi_{1,j}^{n}}{\Delta t} + \alpha_1\delta_x^2\left(\frac{\psi_{1,j}^{n+1} + \psi_{1,j}^{n}}{2}\right) + \frac{S_{1,j}^{n}}{2}\left(\psi_{1,j}^{n+1} + \psi_{1,j}^{n}\right)\right)\overline{\psi_{1,j}^{n+1} - \psi_{1,j}^{n}} = 0. \quad (3.57)$$

The first term in the multiplication (3.57),

$$\frac{i}{\Delta t}\left(\psi_{1,j}^{n+1}-\psi_{1,j}^{n}\right)\left(\overline{\psi_{1,j}^{n+1}}-\overline{\psi_{1,j}^{n}}\right)=\frac{i}{\Delta t}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}}-\psi_{1,j}^{n}\overline{\psi_{1,j}^{n+1}}+\psi_{1,j}^{n}\overline{\psi_{1,j}^{n}}\right)$$
$$=\frac{i}{\Delta t}\left(\left\|\psi_{1,j}^{n+1}\right\|^2+\left\|\psi_{1,j}^{n}\right\|^2-\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}}-\overline{\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}}}\right) \quad (3.58)$$

gives a complex number which is pure imaginary. The second term in the multiplication (3.57) gives

$$\frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j-1}^{n+1}-2\psi_{1,j}^{n+1}+\psi_{1,j+1}^{n+1}+\psi_{1,j-1}^{n}-2\psi_{1,j}^{n}+\psi_{1,j+1}^{n}\right)\left(\overline{\psi_{1,j}^{n+1}}-\overline{\psi_{1,j}^{n}}\right)$$
$$=\frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j-1}^{n+1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j-1}^{n+1}\overline{\psi_{1,j}^{n}}+\psi_{1,j-1}^{n}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j-1}^{n}\overline{\psi_{1,j}^{n}}\right)$$
$$+\frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n}}+\psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n}}\right)$$
$$-\frac{\alpha_1}{\Delta x^2}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}}+\psi_{1,j}^{n}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j}^{n}\overline{\psi_{1,j}^{n}}\right). \quad (3.59)$$

Taking the sum of (3.59) from $j=1$ to $J-1$, shifting the index $j-1$ to j and using the homogenous boundary conditions $\psi_0=\psi_J=0$, we get

$$\frac{\alpha_1}{2\Delta x^2}\sum_{j=1}^{J-2}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n+1}}-\psi_{1,j}^{n+1}\overline{\psi_{1,j+1}^{n}}+\psi_{1,j}^{n}\overline{\psi_{1,j+1}^{n+1}}-\psi_{1,j}^{n}\overline{\psi_{1,j+1}^{n}}\right)$$
$$+\left(\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n+1}}-\psi_{1,0}^{n+1}\overline{\psi_{1,1}^{n}}+\psi_{1,0}^{n}\overline{\psi_{1,1}^{n+1}}-\psi_{1,0}^{n}\overline{\psi_{1,1}^{n}}\right)$$
$$+\psi_{1,J-1}^{n+1}\overline{\psi_{1,J}^{n+1}}-\psi_{1,J-1}^{n+1}\overline{\psi_{1,J}^{n}}+\psi_{1,J-1}^{n}\overline{\psi_{1,J}^{n+1}}-\psi_{1,J-1}^{n}\overline{\psi_{1,J}^{n}}$$
$$-\psi_{1,J-1}^{n+1}\overline{\psi_{1,J}^{n+1}}+\psi_{1,J-1}^{n+1}\overline{\psi_{1,J}^{n}}-\psi_{1,J-1}^{n}\overline{\psi_{1,J}^{n+1}}+\psi_{1,J-1}^{n}\overline{\psi_{1,J}^{n}}$$
$$+\frac{\alpha_1}{2\Delta x^2}\left(\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j+1}^{n+1}\overline{\psi_{1,j}^{n}}+\psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j+1}^{n}\overline{\psi_{1,j}^{n}}\right)$$
$$-\frac{\alpha_1}{\Delta x^2}\left(\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j}^{n+1}\overline{\psi_{1,j}^{n}}+\psi_{1,j}^{n}\overline{\psi_{1,j}^{n+1}}-\psi_{1,j}^{n}\overline{\psi_{1,j}^{n}}\right), \quad (3.60)$$

whose real part is

$$-\frac{\alpha_1}{2}\left(\|(\psi_1)_x^{n+1}\|^2-\|(\psi_1)_x^{n}\|^2\right). \quad (3.61)$$

Similarly, multiply the second equation of (3.47) by $\overline{\psi_{2,j}^{n+1}-\psi_{2,j}^{n}}$ and the third equation of (3.47) by $\overline{\psi_{3,j}^{n+1}-\psi_{3,j}^{n}}$ give

$$-\frac{\alpha_2}{2}\left(\|(\psi_2)_x^{n+1}\|^2-\|(\psi_2)_x^{n}\|^2\right), \quad (3.62)$$

and

$$-\frac{\alpha_3}{2}\left(\|(\psi_3)_x^{n+1}\|^2-\|(\psi_3)_x^{n}\|^2\right). \quad (3.63)$$

respectively.

The nonlinear terms in all multiplications are

$$\frac{1}{2}\left[\sigma\left(\left|\psi_{1,j}^{n+1}\right|^2+\left|\psi_{1,j}^{n}\right|^2\right)+\ e\left(\left|\psi_{2,j}^{n+1}\right|^2+\left|\psi_{2,j}^{n}\right|^2\right)+\sigma\left(\left|\psi_{3,j}^{n+1}\right|^2+\left|\psi_{3,j}^{n}\right|^2\right)\right](\overline{\psi_{1,j}^{n+1}-\psi_{1,j}^{n}}),$$
$$\frac{1}{2}\left[\ e\left(\left|\psi_{1,j}^{n+1}\right|^2+\left|\psi_{1,j}^{n}\right|^2\right)+\sigma\left(\left|\psi_{2,j}^{n+1}\right|^2+\left|\psi_{2,j}^{n}\right|^2\right)+\ e\left(\left|\psi_{3,j}^{n+1}\right|^2+\left|\psi_{3,j}^{n}\right|^2\right)\right](\overline{\psi_{2,j}^{n+1}-\psi_{2,j}^{n}}),$$
$$\frac{1}{2}\left[\sigma\left(\left|\psi_{1,j}^{n+1}\right|^2+\left|\psi_{1,j}^{n}\right|^2\right)+\ e\left(\left|\psi_{2,j}^{n+1}\right|^2+\left|\psi_{2,j}^{n}\right|^2\right)+\sigma\left(\left|\psi_{3,j}^{n+1}\right|^2+\left|\psi_{3,j}^{n}\right|^2\right)\right](\overline{\psi_{3,j}^{n+1}-\psi_{3,j}^{n}}). \quad (3.64)$$

Adding the three terms in (3.64), we get

$$\frac{\sigma\Delta x}{2}\sum_{j=1}^{J-1}\left[\left(\left|\psi_{1,m}^{n+1}\right|^4-\left|\psi_{1,m}^{n}\right|^4\right)+\left(\left|\psi_{2,m}^{n+1}\right|^4-\left|\psi_{2,m}^{n}\right|^4\right)+\left(\left|\psi_{3,m}^{n+1}\right|^4-\left|\psi_{3,m}^{n}\right|^4\right)\right]$$
$$+\,e\Delta x\sum_{j=1}^{J-1}\left(\left|\psi_{2}^{n+1}\right|^2\left|\psi_{3}^{n+1}\right|^2-\left|\psi_{2}^{n}\right|^2\left|\psi_{3}^{n}\right|^2\right)+e\Delta x\sum_{j=1}^{J-1}\left(\left|\psi_{1}^{n+1}\right|^2\left|\psi_{2}^{n+1}\right|^2-\left|\psi_{1}^{n}\right|^2\left|\psi_{2}^{n}\right|^2\right)$$
$$+\,\sigma\Delta x\sum_{j=1}^{J-1}\left(\left|\psi_{1}^{n+1}\right|^2\left|\psi_{3}^{n+1}\right|^2-\left|\psi_{1}^{n}\right|^2\left|\psi_{3}^{n}\right|^2\right) \quad (3.65)$$

Adding (3.61), (3.62), (3.63) and (3.65) and defining E^n as the one in Theorem 3.3.2, we get (3.56). □

3.3.1 Linear Stability Analysis

We note that the difference between the AVF scheme (3.11) and the one–step scheme (3.47) are the nonlinear terms. Application of the one–step scheme (3.47) gives the linear scheme (3.19). Therefore, when we apply linear stability analysis for the one–step scheme (3.47), we get the same results as in the linear stability analysis of the AVF scheme (see Sec.(3.1.1)). Hence, we conclude that, the one-step scheme (3.47) is unconditionally stable in linear sense. According to the Lax theorem the method is convergent, since it is consistent and unconditionally stable [54].

CHAPTER 4

NUMERICAL RESULTS

In this chapter, several test problems are used to show the efficiency and accuracy of the average vector field method (AVF) and the proposed numerical schemes; namely, the two–step method (TSM) (3.28) and the one–step method (OSM) (3.47). Conservation of the mass and the energy are measured by using the error norms

$$\begin{aligned} \|E\|_\infty &= \max_{1\le n\le N}\left|\frac{E^n - E^0}{E^n}\right|, \quad \|Q_k\|_\infty = \max_{1\le n\le N}\left|\frac{Q_k^n - Q_k^0}{Q_k^0}\right|, \\ \|E\|_2 &= \sqrt{\sum_{n=1}^{N}\left|\frac{E^n - E^0}{E^0}\right|^2}, \quad \|Q_k\|_2 = \sqrt{\sum_{n=1}^{N}\left|\frac{Q_k^n - Q_k^0}{Q_k^0}\right|^2}, \end{aligned} \tag{4.1}$$

where $k = 1, 2, 3$ and E^0, Q^0 are the initial discrete energy and the mass, and E^n, Q^n are the discrete energy and the mass at $t = n\Delta t$, respectively. Here E^n is the hamiltonian (3.7). The discrete masses Q_k^n are defined as $\sum_{j=1}^{M} |{\psi_k}_j^n|^2$ for the AVF scheme and the one–step scheme (see (3.49) for one–step scheme). The discrete masses (3.29) are used for the two–step scheme. We solved the problem (2.2)–(2.3) on the spatial domain $[x_L, x_R]$ and the temporal domain $[0, T]$ with the spatial step length $\Delta x = (x_R - x_L)/M$ and temporal step size $\Delta t = t/N$. Here M and N represents spatial and temporal grid points, respectively. While the periodic boundary conditions

$$\psi_k(x_L, t) = \psi_k(x_R, t), \quad k = 1, 2, 3$$

are used for the AVF method (3.11) and the two step scheme (3.28), homogenous boundary conditions

$$\psi_k(x_L, t) = \psi_k(x_R, t) = 0, \quad k = 1, 2, 3$$

are used for the one step method (3.47). In all computations we choose $\alpha_1 = \alpha_2 = \alpha_3 = 1$ and $\sigma = 1$. In all figures the surfaces obtained by using the AVF scheme are shown because the surfaces obtained by the one–step method and the two–step method are identical. The nonlinear system of equations obtained by the AVF method and the one–step (OSM) methods are solved by using Newton method at each time step with an error tolerance 10^{-7} as described in Section (3.1).

To advance the solution from t_{n+1} to t_n while AVF method requires two iterations, the one–step (OSM) method requires three iterations in Newton method. We get similar result for different error tolerance such as 10^{-15}. For this point of view we can say that the AVF method is slightly better than the OSM. The advantage of the two–step method (TSM) with respect to the AVF method and one step method (OSM) is that it is globally linear implicit, which means that at each discrete time level we only need to solve a set of linear algebraic equations to get $\psi_{k,j}^{n+1}$.

4.1 Periodic Wave Solution

In the first test we will look at the evolution of unstable periodic wave of the 3-CNLS equation (2.2) with $e = 1$, $[x_L, x_R] = [-4\pi, 4\pi]$ and $M = 128$. The following initial conditions are used [61]

$$\begin{aligned} \psi_1(x) &= a_0[1 - \varepsilon\cos(\ell x)], \\ \psi_2(x) &= b_0[1 - \varepsilon\cos(\ell(x+\theta))], \\ \psi_3(x) &= c_0[1 - \varepsilon\cos(\ell x)], \end{aligned} \tag{4.2}$$

where a_0, b_0 and c_0 are the initial amplitudes of the perturbed waves. A small parameter $\varepsilon \ll 1$ represents the strength of perturbation, ℓ is the wave number of the perturbation and θ is the phase difference. A periodic wave is a wave that repeats itself regularly in an interval. They are characterized by amplitude, frequency and wavelength. Length scale of a periodic wave in a spatial domain means wavelength. Time scale of periodic wave in time domain means period. More often frequency is used instead of period in order to characterize the periodic wave which represents the number of waves repeats in a second.

The following parameters are used in the test:

$$a_0 = 0.2, b_0 = 0.3, c_0 = 0.2,\ \varepsilon = 0.1,\ \ell = 0.5,\ \theta = 0.$$

It is known that the plane wave is stable if $\ell_c \geq \sqrt{2\left(a_0^2 + b_0^2 + c_0^2\right)}$ [61]. The choice of $\ell = 0.5$ implies that the plane wave (4.2) is unstable. We solved the problem (2.2) with $\Delta t = 5 \times 10^{-3}$ and compare the AVF method (3.11), the two–step scheme (3.28) and the one–step scheme (3.47) with the Exponential time differencing Crank–Nicolson (ETD–CN) method with a quartic spline interpolation approximation [64] and the multisymplectic six-point scheme [61]. For comparative purpose we compute $||\psi_1||_2^2$ and $||\psi_2||_2^2$ and used the same error $\left| ||\psi(\cdot, T)||_2^2 - ||\psi(\cdot, 0)||_2^2 \right|$ as in [64]. Since the value of $||\psi_3||_2^2$ is same with $||\psi_1||_2^2$, it is not presented in the test. According to the initial values (4.2), the exact values of $||\psi_1||_2^2$ and $||\psi_2||_2^2$ at $t = 0$ are 1.00515481265051 and 1.50773221897576, respectively. From the Table 4.1 we see that the two–step scheme (3.28) and one–step scheme (3.47) conserve the masses $||\psi_j||_2^2$, $j = 1, 2$ exactly. Moreover, the AVF scheme (3.11) preserves the mass better than the multisymplectic six–point scheme [61] and the Exponential time differencing Crank–Nicolson (ETD–CN) method with a quartic spline interpolation approximation [64]. Figure 4.1 represents surfaces of the waves ψ_1 and ψ_2. The surface of ψ_3 is identical to the surface of ψ_1, for this reason it is not

Table 4.1: Periodic Wave Solution. Errors in conservations of $||\psi_j||_2^2$, $j = 1, 2$ via the multisymplectic six–point scheme [61], the Exponential time differencing Crank–Nicolson (ETD–CN) method with a quartic spline interpolation approximation [64]

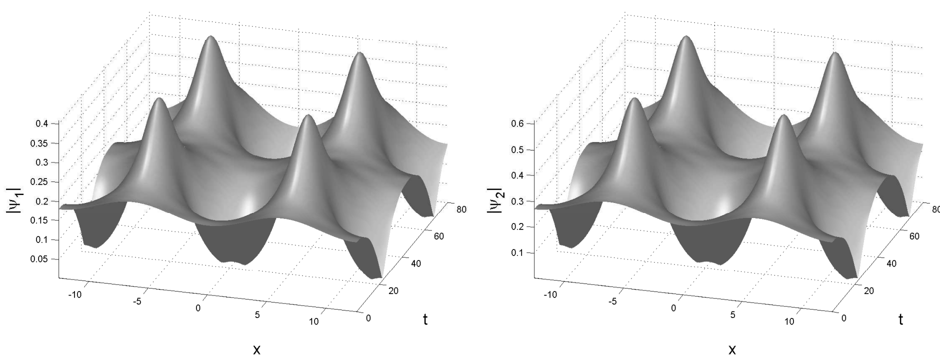
	$\|\|\psi_1\|\|_2^2$		$\|\|\psi_2\|\|_2^2$	
	$T = 20$	$T = 80$	$T = 20$	$T = 80$
Error in [61]	$5.7e-04$	$3.2e-05$	$8.7e-04$	$8.0e-05$
Error in [64]	$1.1e-05$	$2.2e-05$	$5.4e-05$	$6.0e-05$
Error in AVF	$1.4e-07$	$9.4e-09$	$2.2e-07$	$1.4e-08$
Error in TSM	$2.5e-14$	$1.0e-13$	$3.8e-14$	$1.4e-13$
Error in OSM	$3.6e-14$	$1.1e-13$	$7.5e-14$	$1.6e-13$

shown in the figure. From the figure we see that while the wave of ψ_1 has its amplitude around 0.4, the amplitude of the other wave ψ_2 is around 0.6. There are two peaks within the length of spatial domain. All schemes well simulate the periodic wave.

Figure 4.2 represents the effect of phase difference in the surface of the destabilized periodic waves. Notice that changing the value of the phase difference $\theta = 0$ with $\theta = 7\pi/4$ in ψ_2 yields a decrease in the number of peaks in ψ_1. Because the system is coupled, the evolution of the wave ψ_2 effects the evolution of ψ_1 and ψ_3.

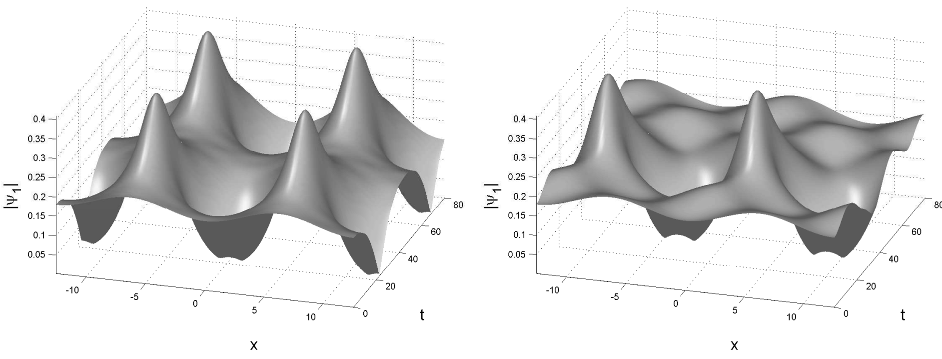
Tables 4.2– 4.4 shows the mass conservations at various times. These tables verify the theoretical result in Section 3.2 and Section 3.3 that the two–step scheme and one–step scheme are mass conserving.

In addition, we see that the AVF scheme preserves the mass quite well. Table 4.5 represents energy errors for the proposed methods. The table verifies the theoretical result in Section 3.1 and Section 3.3 that the AVF scheme and the one step scheme are energy preserving. It can be seen that the one–step



(a) ψ_1 (b) ψ_2

Figure 4.1: Surfaces of destabilized wave solutions of the 3−CNLS equation (2.2) with $\ell = 0.5$ and $\theta = 0$



(a) $\theta = 0$ (b) $\theta = 7\pi/4$

Figure 4.2: Effect of the phase difference on the surface of ψ_1.

Table 4.2: Periodic Wave Solution. Mass conservation of 3−CNLS equation (2.2) via the AVF method with $M = 128$ and $\Delta t = 0.005$

T	$\|\|\psi_1\|\|_2^2$	Error	$\|\|\psi_2\|\|_2^2$	Error	$\|\|\psi_3\|\|_2^2$	Error
0	1.0051	0.0000	1.5077	0.0000	1.0051	0.0000
20	0.200342	$2.6e-6$	0.446248	$0.03e-6$	0.200342	$2.6e-6$
50	0.200342	$6.3e-6$	0.446248	$1.4e-6$	0.200342	$6.3e-6$
80	0.200342	$9.0e-6$	0.446248	$2.0e-6$	0.200342	$9.0e-6$

Table 4.3: Periodic Wave Solution. Mass conservation of 3−CNLS equation (2.2) via the two step method with $M = 128$ and $\Delta t = 0.005$

T	$\|\|\psi_1\|\|_2^2$	Error	$\|\|\psi_2\|\|_2^2$	Error	$\|\|\psi_3\|\|_2^2$	Error
0	1.0051	0.000	1.5077	0	1.0051	0.000
20	0.396663	$1.9e-11$	0.892477	$1.9e-11$	0.396663	$1.9e-12$
50	0.396663	$6.6e-12$	0.892477	$6.6e-12$	0.396663	$6.6e-12$
80	0.396663	$6.7e-12$	0.892477	$6.7e-12$	0.396663	$6.7e-12$

Table 4.4: Periodic Wave Solution. Mass conservation of 3−CNLS equation (2.2) via the one step method with $M = 128$ and $\Delta t = 0.005$

T	$\|\|\psi_1\|\|_2^2$	Error	$\|\|\psi_2\|\|_2^2$	Error	$\|\|\psi_3\|\|_2^2$	Error
0	1.0051	0.0000	1.5077	0	1.0051	0.0000
20	0.197085	$3.6e-14$	0.446248	$7.5e-14$	0.197085	$7.0e-14$
50	0.197085	$8.0e-14$	0.446248	$1.9e-13$	0.197085	$8.3e-14$
80	0.197085	$1.1e-13$	0.446248	$1.6e-13$	0.197085	$9.0e-14$

method (3.47) gives more accurate results than the AVF method (3.11).

4.2 Soliton Solution

Solitary wave or a soliton is a wave which does not change its shape in long time period. It has been first experimentally observed by John Scott Russell on the Edinburgh–Glasgow water channel

Table 4.5: Periodic Wave Solution. Errors in energy with $M = 128$ and $\Delta t = 0.005$

T	$\|\|E_{AVF}\|\|_\infty$	$\|\|E_{AVF}\|\|_2^2$	$\|\|E_{OSM}\|\|_\infty$	$\|\|E_{OSM}\|\|_2^2$	$\|\|E_{TSM}\|\|_\infty$	$\|\|E_{TSM}\|\|_2^2$
0	0	0	0	0	0	0
20	$7.7e-12$	$3.1e-10$	$4.5e-16$	$9.2e-15$	$2.4e-5$	$6.8e-4$
50	$2.0e-11$	$1.1e-9$	$7.9e-16$	$2.3e-14$	$2.4e-5$	$9.9e-4$
80	$3.2e-11$	$2.4e-9$	$7.7e-15$	$2.9e-13$	$2.4e-5$	$1.4e-3$

in 1845 [1, 2]. The solitary wave theory has been an important subject after this date. The popularity of soliton still in progress in wide range of research areas such as classical and quantum theory, fluid mechanics, nonlinear optics and plasma physics in applied mathematics and physics [68]. Many nonlinear equation models such as Korteweg–de Vries (KdV) equation, NLS equation, 2-CNLS equation and Sine–Gordon equation have soliton solutions. Russell stated the following facts about solitary waves [68]:

- a solitary wave has a hyperbolic secant shape and travel with permanent velocity and form.
- soliton can interact with each other without change of any kind.
- a sufficiently large initial mass of water produces two or more independent solitary waves.
- larger amplitude waves move faster than the smaller amplitude waves.

Therefore, in a conservative system amplitude, shape and velocity of a solitary wave should be preserved after colliding (interaction) of two or more soliton [68]. A simple form of the solitary wave can be expressed as

$$u(x,t) = sech(x - ct), \quad c \in \mathbb{R}.$$

In this section, the evolution of solitary wave solution of the 3−CNLS equation will be investigated to authenticate the adaptability and accuracy of the presented methods.

4.2.1 One Soliton Solution

First, we will consider the one soliton solution for the system (2.2). The problem is solved in the region $(x,t) \in x[-20, 60] \times [0, 10]$ with temporal step size $\Delta t = 0.01$ and spatial step size $\Delta x = 0.3$. The initial conditions

$$\psi_k(x,0) = \frac{1}{\sqrt{3}} sech(x)\, e^{ix}, \quad k = 1,2,3 \tag{4.3}$$

are used in this test. The initial condition (4.3) represent a solitary wave located at the spatial position $x = 0$ with the amplitude $1/\sqrt{3}$ as shown in Figure 4.3. Note that the initial data decay sufficiently rapidly as $|x| \to \infty$ which plays an important role in conservation properties of 3−CNLS, as described

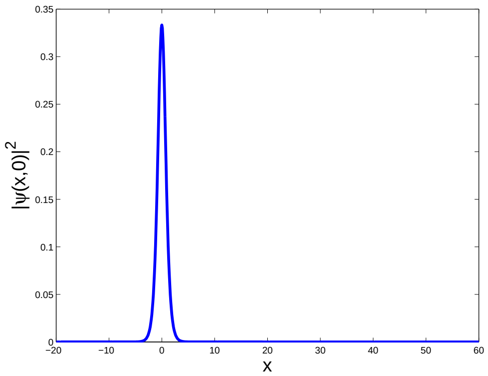
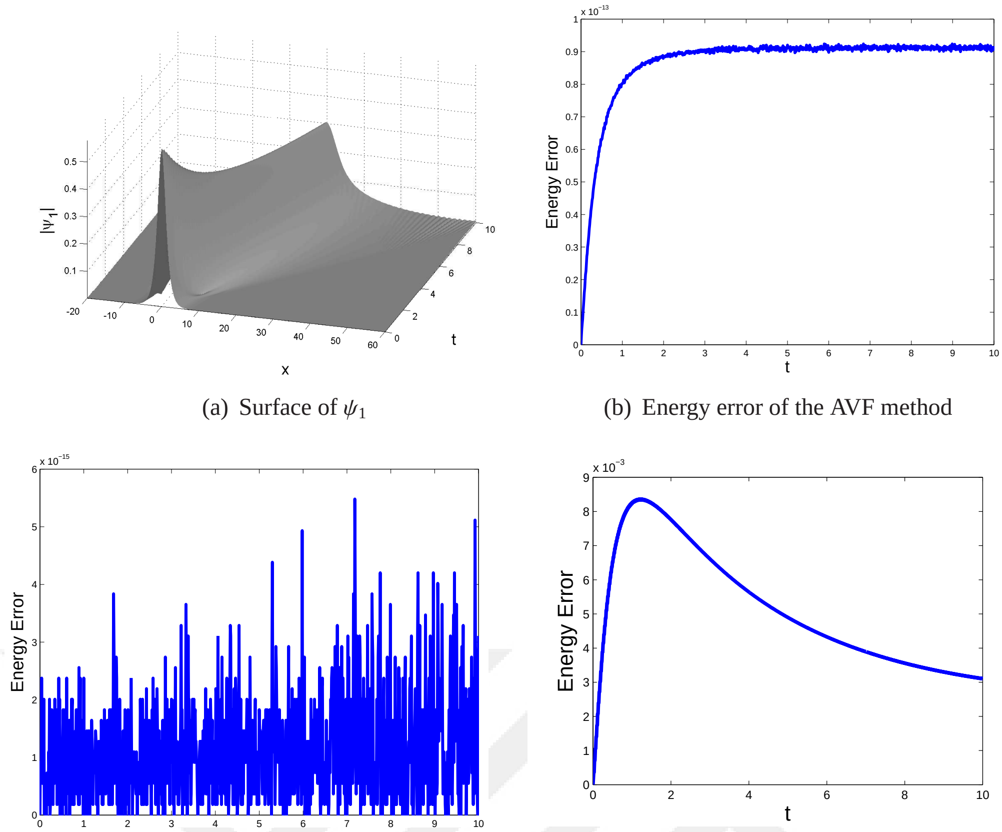


Figure 4.3: Initial profile of single soliton

Table 4.6: One Soliton Solution. Errors in mass and energy conservations

Method	$\|\|Q_1\|\|_2$	$\|\|Q_1\|\|_\infty$	$\|\|E\|\|_2$	$\|\|E\|\|_\infty$
AVF	$1.370e-4$	$5.300e-6$	$2.774e-12$	$9.238e-14$
OSM	$1.848e-14$	$2.331e-15$	$4.484e-14$	$5.481e-15$
TSM	$4.591e-14$	$4.329e-15$	0.17179	0.008363

in Section 2.1. The spatial domain $-20 \leq x \leq 60$ is chosen large enough so that boundaries do not affect the the solitary wave propagation in numerical simulation. To study the behavior of the proposed schemes, we choose $e = 1$. The errors in conserved quantities; namely, the mass Q_1 and the energy E are displayed in Table 4.6. The errors in conservations of the masses Q_2 and Q_3 are similar, therefore not shown in the table. The table verifies the theoretical results in previous sections that the AVF method is energy preserving, two–step method is mass preserving and the one step method is both energy and mass preserving method. Although the AVF method is energy preserving, we see that it preserves the mass quite well. Figure 4.4(a) represents the behavior of the one soliton at the time $t = 10$. We see that solitary wave is moving to the right. In Figures 4.4(b), 4.4(c) we se that energy is exactly preserved by the AVF method (3.11) and the one-step method (3.47). Although the energy error for the AVF scheme increases at the beginning of the simulation, it remains constant after $t \approx 2$. While the energy error of the AVF scheme is about 10^{-13}, the energy error of the one step method is about 10^{-15}. This shows that the one-step method is more efficient than the AVF scheme with respect to the energy preservation.



(a) Surface of ψ_1 (b) Energy error of the AVF method

(c) Energy error of one step method (d) Energy error of two step method

Figure 4.4: One soliton solution for $e = 1$: Surface and errors

4.2.2 Three Solitons Solution

We consider the 3–CNLS equation (2.2) with the initial condition

$$\begin{aligned} \psi_1(x,0) &= \sqrt{2}r_1 \mathrm{sech}(r_1 x + x_{10}) e^{iv_1 x}, \\ \psi_2(x,0) &= \sqrt{2}r_2 \mathrm{sech}(r_2 x - x_{20}) e^{-iv_2 x}, \\ \psi_3(x,0) &= \sqrt{2}r_3 \mathrm{sech}(r_3 x + x_{30}) e^{iv_3 x}, \end{aligned} \tag{4.4}$$

to see the evolution of solitary wave solution. In the initial condition (4.4), $\psi_1(x,0)$ represents a solitary wave located initially at the position x_{10} with velocity v_1.

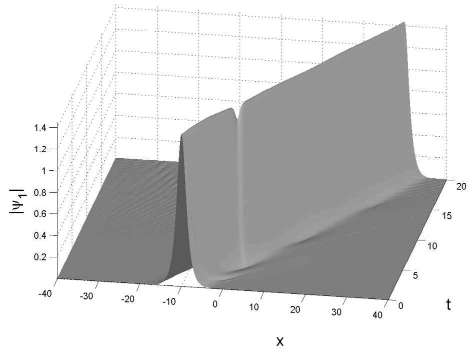
4.2.2.1 Elastic collision ($e = 1$):

We consider the 3−CNLS equation (2.2) in the region $-40 \leq x \leq 40$ so that the the boundaries do not effect the solitary wave propagation. We take $M = 400$, $\Delta t = 0.02$, $r_1 = r_2 = r_3 = 1.0$, $v_1 = v_2 = 1.0$, $v_3 = 1/4$, $x_{10} = x_{20} = 10$ and $x_{30} = 30$. Table 4.7 displays some errors corresponding to the AVF scheme (3.11), the two–step scheme (3.28) and the one–step scheme (3.47), for various space and time steps. It can be seen from the Table 4.7 that schemes produce remarkable reduction in the

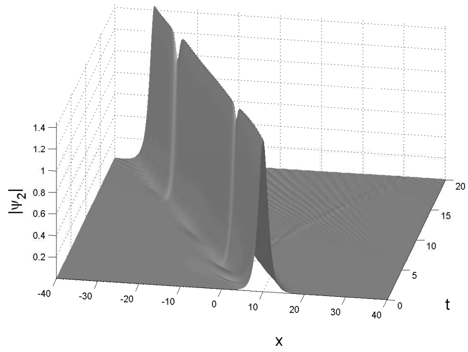
Table 4.7: Accuracy in solitary wave solution for $e = 1$ at time $T = 1$.

	Δx	Δt	$\|\|Q_1\|\|_\infty$	$\|\|Q_2\|\|_\infty$	$\|\|Q_3\|\|_\infty$	$\|\|E\|\|_\infty$
AVF	0.25	0.25	$1.0e-3$	$1.3e-3$	$4.6e-5$	$3.8e-10$
		0.125	$7.9e-5$	$7.9e-5$	$1.3e-5$	$1.2e-11$
		0.0625	$6.1e-6$	$6.1e-6$	$1.3e-6$	$2.6e-11$
	0.125	0.125	$6.1e-5$	$6.1e-5$	$2.7e-6$	$2.3e-10$
		0.0625	$5.2e-6$	$5.2e-6$	$8.2e-7$	$4.9e-11$
TSM	0.25	0.25	$1.1e-15$	$1.1e-15$	$1.9e-15$	$7.1e-1$
		0.125	$1.7e-15$	$8.8e-16$	$1.3e-15$	$3.8e-1$
		0.0625	$4.4e-16$	$2.2e-16$	$4.4e-16$	$1.3e-1$
	0.125	0.125	$9.7e-15$	$5.1e-15$	$5.1e-15$	$3.2e-1$
		0.0625	$2.8e-15$	$1.5e-15$	$2.2e-15$	$1.7e-1$
OSM	0.25	0.25	$1.1e-15$	$1.1e-15$	$3.3e-16$	$1.5e-15$
		0.125	$4.4e-16$	$4.4e-16$	$6.6e-16$	$3.0e-15$
		0.0625	$6.6e-16$	$6.6e-16$	$1.1e-15$	$2.8e-15$
	0.25	0.125	$6.6e-16$	$6.6e-16$	$1.2e-15$	$2.5e-15$
		0.0625	$6.6e-16$	$6.6e-16$	$1.1e-15$	$3.3e-15$

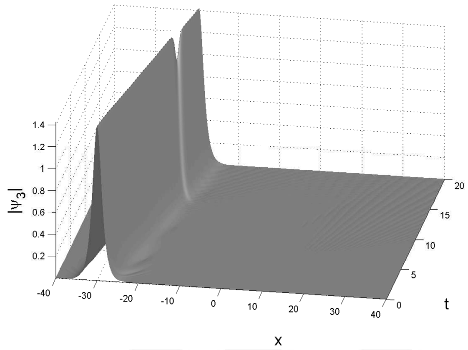
errors when the step sizes are reduced and convergence is evident. Figure 4.5 (a–c) represents the evolution of solitary waves for $0 \leq t \leq 20$ and $e = 1$. From the figure wee see that the waves ψ_1 and ψ_3 moves to the right, while the wave ψ_2 moves to the left in time. The wave ψ_1 collides to the wave ψ_2 about the time $t \approx 3$, and the wave ψ_3 collides to the wave ψ_2 about the time $t \approx 15$. During collision we observe a decrease in the amplitudes of the waves, but after the collision there is a roundup in the amplitudes. We see that after collisions, the waves moves forward in the same direction and three waves emerge without change in their shapes and velocities. This shows that the collision is elastic. In the context of biophysics, the Figure 4.5 shows the interaction of three solitons during theirs propagation through the alpha helical protein chain [69]. From the Figure 4.5(d), we can conclude that the total energy of the three solitons are found to be conserved and there is no change in the distribution of energy among them in the neighboring spines keeping the total energy conserved. Table 4.8 shows the errors in conservation properties the masses and the energies. The table verifies the expected results that the AVF scheme preserves the energy, the two–step method preserves the masses, and the one–step method preserves both mass and energy. Figure 4.6 represents the errors in elastic collision. In addition to the Table 4.8, the Figure 4.6 verifies the same theoretical results presented in Chapter 3. Again, we see that one–step method (OSM) preserves the energy and the masses better than AVF and two–step method (TSM).



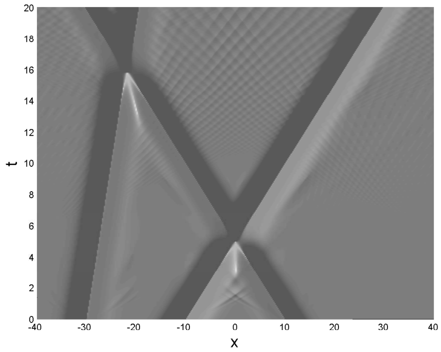
(a) Surface $|\psi_1|$



(b) Surface $|\psi_2|$



(c) Surface $|\psi_3|$



(d) Surface $|\psi_1| + |\psi_2| + |\psi_3|$

Figure 4.5: Three solitons solution for $e = 1$

4.2.2.2 Creation of new vector soliton ($e = 2$) and fusion ($e = 0.35$)

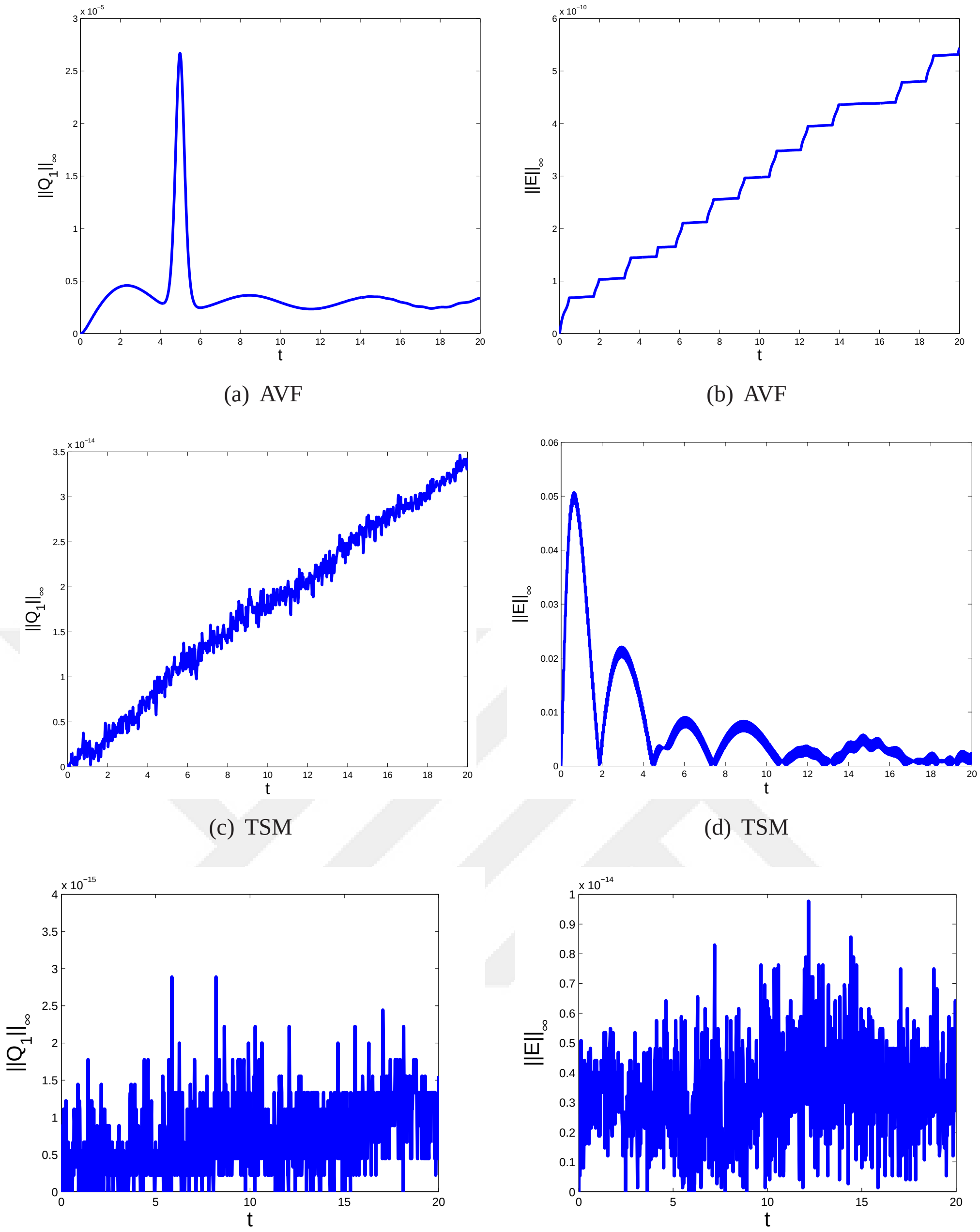
In this test, we present creation of new vector soliton and fusion scenarios of three solitary wave solutions. First, we choose the wave-wave interaction coefficient $e = 2$. The following parameters are used in this test:

$$r_1 = 1.0,\ r_2 = 1.2,\ r_3 = 1.3,\ v_1 = 1/4,\ v_2 = 1/4,\ v_3 = 1/2,\ x_{10} = x_{20} = 10,\ x_{30} = 30.$$

Figure 4.7 represents the contour plot over the spatial domain $-40 \leq x \leq 40$ up to $T = 29$ for

Table 4.8: Errors in solitary wave solution for $e = 1$

		$\|\|Q_1\|\|_\infty$	$\|\|Q_2\|\|_\infty$	$\|\|Q_3\|\|_\infty$	$\|\|E\|\|_\infty$
AVF	$T = 10$	$2.67e - 5$	$2.67e - 5$	$7.77e - 7$	$2.97 - 10$
	$T = 20$	$2.67e - 5$	$2.67e - 5$	$6.36e - 5$	$5.44 - 10$
TSM	$T = 10$	$1.97e - 14$	$1.77e - 14$	$1.99e - 14$	$5.70 - 02$
	$T = 20$	$3.46e - 14$	$3.19e - 14$	$3.64e - 14$	$5.07 - 02$
OSM	$T = 10$	$2.88e - 15$	$2.22e - 15$	$2.44e - 15$	$8.29e - 15$
	$T = 20$	$2.88e - 15$	$3.10e - 15$	$2.88e - 15$	$9.76e - 15$



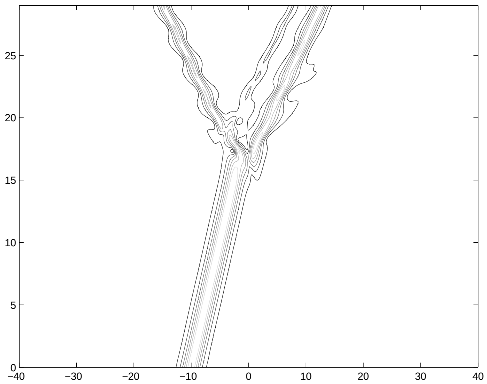
(a) AVF (b) AVF

(c) TSM (d) TSM

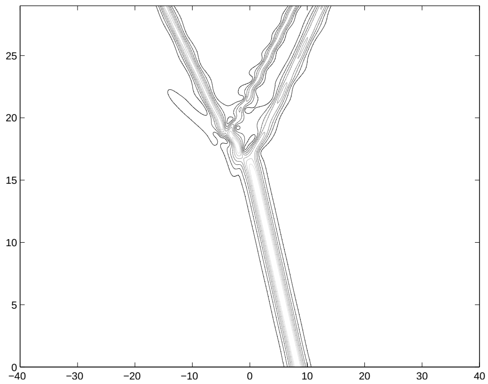
(e) OSM (f) OSM

Figure 4.6: Errors in three solitons solution for $e = 1$

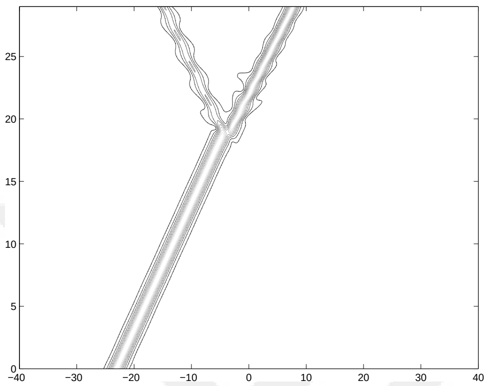
the values $M = 400$ and $\Delta t = 0.01$. From the figure, we see that the collisions takes place between the time interval $15 \leq t \leq 20$. We can see the creation of new vector soliton after the collision of three soliton. Figure 4.8 represents the error in mass conservation and the energy conservation in the collision. From the figure, we can see that mass errors in the numerical solutions are very small. Therefore, we can say that creation of new vector soliton is not the consequence of numerical errors. We note that collision take place about the time $t \approx 15$. We can see that after the collision there is a violation in the preservation of the energy by the AVF method and the one–step method. The errors in mass conservation by the two–step method are within the limits of the round–off error of machine.



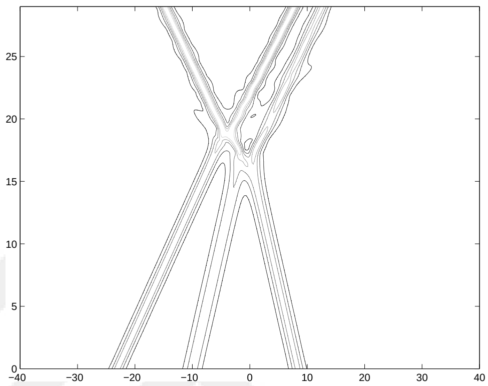
(a) Contour $|\psi_1|$



(b) Contour $|\psi_2|$



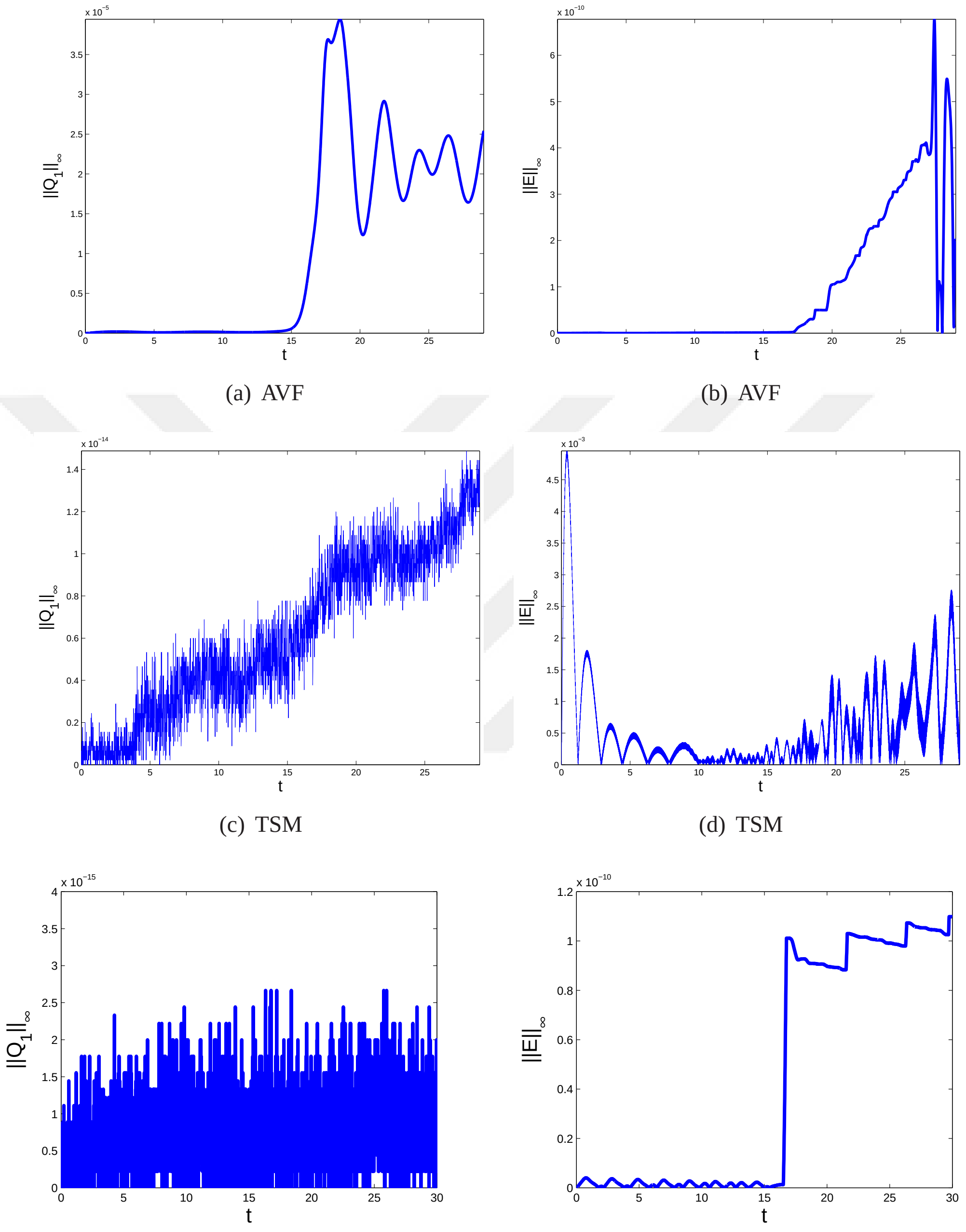
(c) Contour $|\psi_3|$



(d) Contour $|\psi_1| + |\psi_2| + |\psi_3|$

Figure 4.7: Three solitons solution. Creation of vector soliton for $e = 2$

If we change the wave–wave interaction coefficient e and choose $e = 0.35$ we observe the fusion of three soliton in Figure 4.9. The errors in the fusion scenario are shown in the Figure 4.10. Figures 4.8 and 4.10 verify the energy and mass conservation in the proposed methods presented in the Chapter 3.

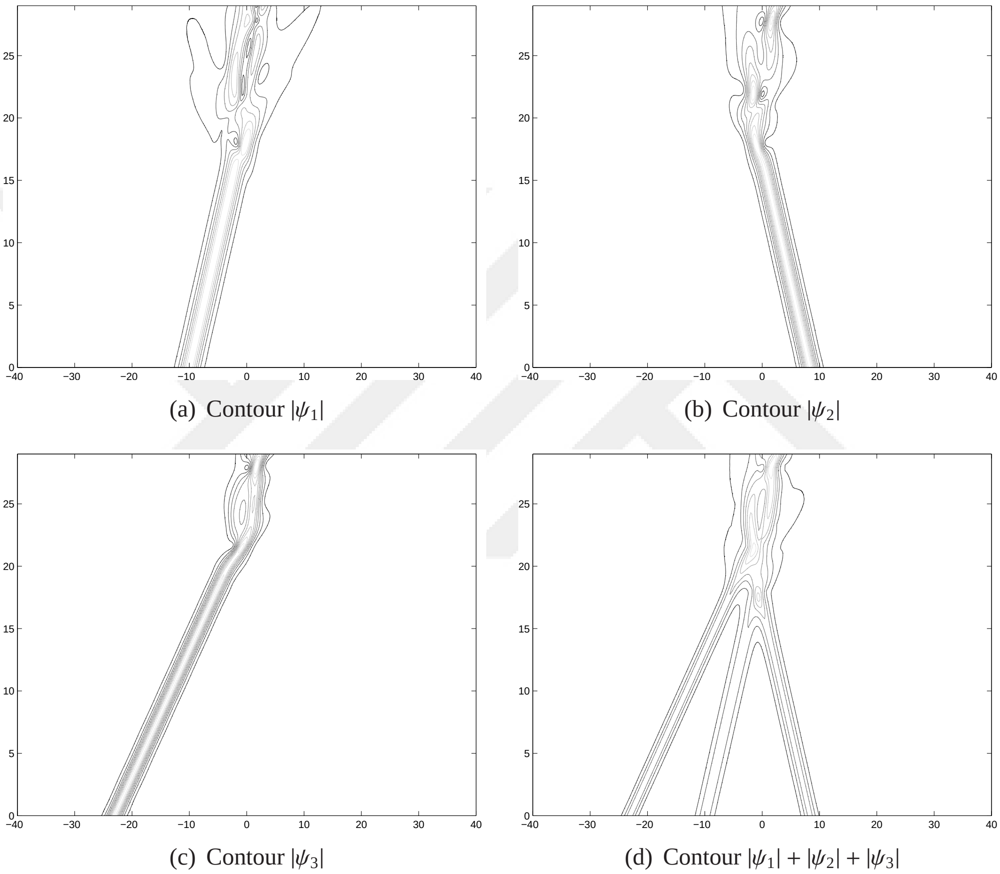


(a) AVF (b) AVF

(c) TSM (d) TSM

(e) OSM (f) OSM

Figure 4.8: Three solitons solution. Errors in creation of vector soliton for $e = 2$



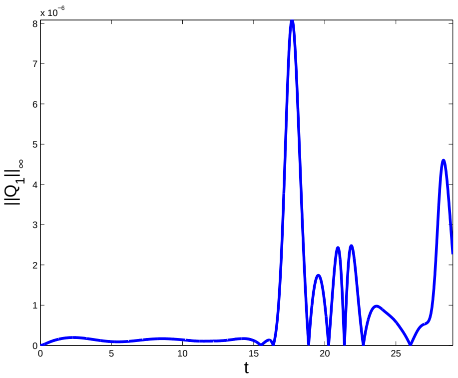
(a) Contour $|\psi_1|$

(b) Contour $|\psi_2|$

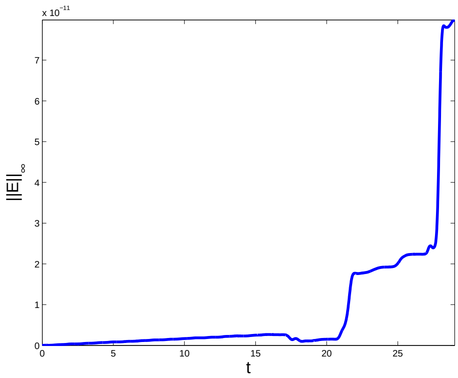
(c) Contour $|\psi_3|$

(d) Contour $|\psi_1| + |\psi_2| + |\psi_3|$

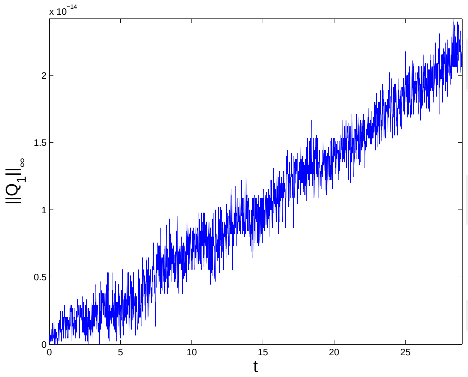
Figure 4.9: Three solitons solution. Fusion of three solitons for $e = 0.35$



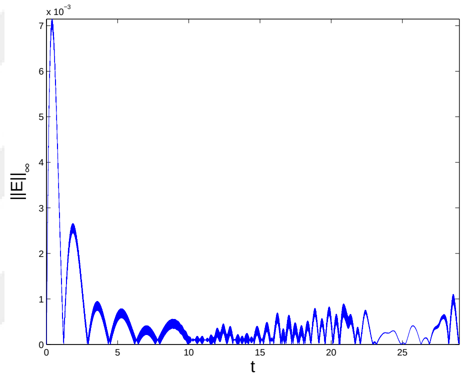
(a) AVF



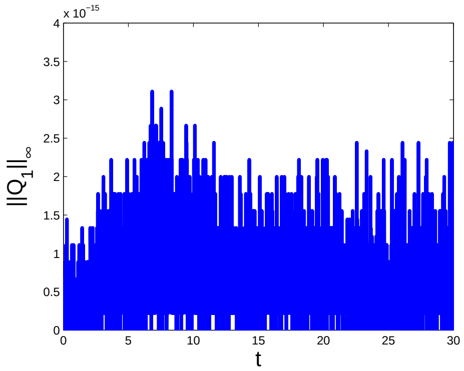
(b) AVF



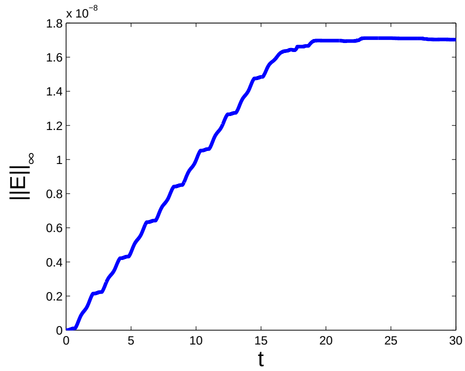
(c) TSM



(d) TSM



(e) OSM



(f) OSM

Figure 4.10: Three solitons solution. Errors in fusion of three solitons for $e = 0.35$

CHAPTER 5

DISPERSION RELATION

In the previous chapter, we have proposed three different finite difference schemes for the numerical solution of the 3–CNLS equation (2.2). In addition, we have discussed qualitative behavior of the schemes such as conservation of mass and/or energy of the 3–CNLS equation. There are many different nonlinear wave equations. Some types of equations have solutions that display singularities and solutions blow–up, while some type of equations have dispersive solutions, i.e. solutions decaying in time and space. The preservation of energy and/or mass can not give sufficient information about the numerical methods. In particular, if the equation is dispersive, dispersive property of the numerical solution gives valuable information about the long time integration of the scheme. In this chapter, we will discuss another useful tool that can be used to check how well the numerical method works. The use of relatively simple solution

$$u(x,t) = \hat{u}e^{i(\xi x - \omega t)}, \qquad i = \sqrt{-1} \tag{5.1}$$

is an important tool for analyzing wave problems. The solution (5.1) is called plane wave solution [70]. It describes a wave in space x and time t. In the expression (5.1), ξ is the wave number, ω is the frequency of the wave and $\hat{u}$ is the amplitude of the wave. The number $\lambda = 2\pi/\xi$ is the wave length. Unless stated otherwise stated it is assumed that $0 < \xi < \infty$. In (5.1), $u(x,t)$ represents a sinusoidal wave of length $2\pi/\xi$, period $2\pi/\omega$ and phase velocity ω/ξ.

In this chapter, we will investigate the numerical dispersion of the proposed schemes to understand the behavior of the numerical solutions. Approximating the nonlinear partial differential equation by the linearized one, we can determine the behavior of the nonlinear PDE by dispersion relation. Since the exact solution of the linear PDE can be found, we can make a comparison of the continuous solution with the numerical solution, applied to the linear PDE, via dispersion relation. So, we will consider the linearized 3–CNLSE using the methods given in (3.11), (3.47) and (3.28), and then compare the dispersion relations for the discrete and continuous versions of the equation.

The dispersion relation provides the relationship between the wave number ξ and the frequency ω of the modes (or ”wave”). The dispersion relation can be written as

$$\omega = \omega(\xi). \tag{5.2}$$

Each wave number ξ corresponds to m frequencies ξ, where m is the order of the differential equation with respect to t, that is why (5.2) is called as a relation rather than a function.

Assume that $u(x,t)$ is a function with an unbounded domain and it satisfies a linear partial differential equation with constant coefficients. Then, it has a solution of the form [70]

$$u(x,t) = \int_{-\infty}^{\infty} A(\xi) e^{i(\xi x - \omega(\xi)t)} d\xi, \tag{5.3}$$

where $A(\xi)$ is an arbitrary function.

Suppose that each wave itself is a solution of the linear PDE, then the solution takes the form:

$$u(x,t) = \hat{u} e^{i(\xi x - \omega(\xi)t)}, \tag{5.4}$$

where $\hat{u}$ is constant. Typically $\omega = Re(\omega) + iIm(\omega) = \omega_r + i\omega_i$, then the equation (5.4) can be written as

$$u(x,t) = \hat{u} e^{i(\xi x + \omega_r t)} e^{-\omega_i t}. \tag{5.5}$$

We see that whenever the frequency ω is purely imaginary, the plane wave (5.1) will either grow or decay in time. In particular

- If $\omega_i > 0$, then the plane wave will decay,
- If $\omega_i < 0$, then the plane wave will grow without a bound.

In the case when ω is real, the plane wave (5.1) will be in the form

$$u(x,t) = \hat{u} e^{i(\xi x + \omega_r t)}$$

and the wave will propagate with speed ω/ξ and with no decay of amplitude (see the top figure in Figure 5.1). When ω is imaginary, there will be grow or decay in the plane wave according to sign of imaginary term (see the bottom figure in Figure 5.1). The decay or grow of the solution is an important part of the behavior of the solution of PDE. If the Fourier modes do not grow with time and if at least one mode decays, then the PDE is said to be dissipative. When the Fourier modes neither decay nor grow, then the PDE is called non–dissipative. The PDE is called dispersive when Fourier modes of different wave lengths (or wave numbers) propagate at different speeds. In practice, PDE containing only even ordered x derivatives are dissipative. PDE containing only odd ordered x derivatives is non-dissipative and when the order is greater than one the PDE is dispersive. One of the

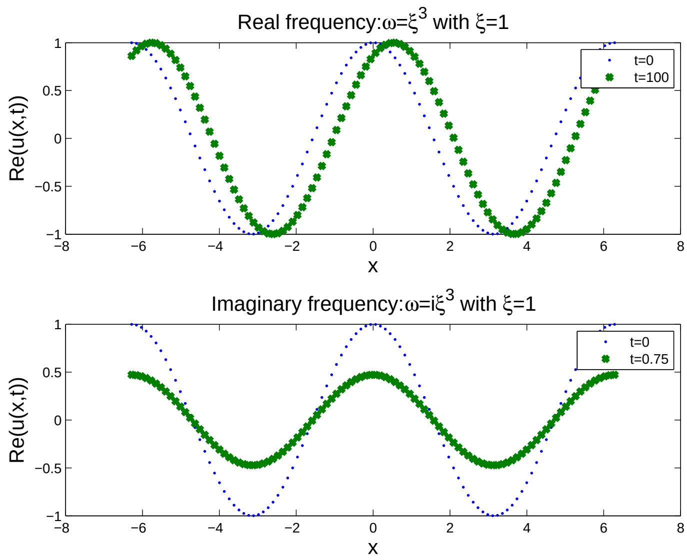


Figure 5.1: Plane waves with pure real part or pure imaginary part

important analysis for numerical schemes is to see if the difference schemes have the same dissipative or dispersive properties with the corresponding PDE [70].

This chapter is devoted to discussion of dispersion relation of the linearized 3–CNLS equation and the corresponding numerical dispersion relations. From the Figure 5.1 we see that the plane wave is simple periodic wave. Since we have used periodic boundary conditions for the energy conserving AVF method and the mass conserving two–step method, we will analyze the numerical dispersion relations of those schemes. Plane wave analysis of the one–step method can not give any valuable information about the behavior of solution because we have used homogenous boundary conditions for this method.

5.1 Continuous Dispersion Relation

We begin the discussion of dispersion analysis by considering the linear 3–CNLS equation (2.2) with $\alpha_1 = \alpha_2 = \alpha_3 = 1$ in the form,

$$\begin{aligned} i\psi_{1t} + \psi_{1xx} + c_1\psi_1 &= 0, \\ i\psi_{2t} + \psi_{2xx} + c_2\psi_2 &= 0, \\ i\psi_{1t} + \psi_{3xx} + c_1\psi_3 &= 0, \end{aligned} \tag{5.6}$$

where the constants c_1 and c_2 are [49, 53]

$$\begin{aligned} c_1 &= \max_{x_L \le x \le x_R,\ 0 \le t \le T} \left(\sigma|\psi_1|^2 + e|\psi_2|^2 + \sigma|\psi_3|^2 \right), \\ c_2 &= \max_{x_L \le x \le x_R,\ 0 \le t \le T} \left(e|\psi_1|^2 + \sigma|\psi_2|^2 + e|\psi_3|^2 \right). \end{aligned}$$

The linear equations (5.6) admits plane wave solution of the form

$$\psi_1(x,t) = e^{i(\xi_1 x - \omega_1 t)},\ \psi_2(x,t) = e^{i(\xi_2 x - \omega_2 t)},\ \psi_1(x,t) = e^{i(\xi_3 x - \omega_3 t)}. \tag{5.7}$$

Substituting them into (5.6) yields

$$\begin{aligned} i(-i\omega)e^{i(\xi_1 x-\omega_1 t)} + (i\xi_1)^2 e^{i(\xi_1 x-\omega_1 t)} + c_1 e^{i(\xi_1 x-\omega_1 t)} &= 0,\\ i(-i\omega)e^{i(\xi_2 x-\omega_2 t)} + (i\xi_2)^2 e^{i(\xi_2 x-\omega_2 t)} + c_2 e^{i(\xi_2 x-\omega_2 t)} &= 0,\\ i(-i\omega)e^{i(\xi_3 x-\omega_3 t)} + (i\xi_3)^2 e^{i(\xi_3 x-\omega_3 t)} + c_1 e^{i(\xi_3 x-\omega_3 t)} &= 0. \end{aligned} \tag{5.8}$$

Canceling the exponential terms $e^{i(\xi_k x-\omega_k t)}$, $k = 1,2,3$ respectively, we get the dispersion relations

$$\omega_1 = \xi_1^2 - c_1,\ \omega_2 = \xi_2^2 - c_2,\ \omega_3 = \xi_3^2 - c_1. \tag{5.9}$$

For these dispersion relations, the plane wave solution (5.7) becomes

$$\begin{aligned} \psi_1(x,t) &= e^{i(\xi_1 x-\omega_1 t)} = e^{i\xi_1 x}e^{-i(\xi_1^2-c_1)t},\\ \psi_2(x,t) &= e^{i(\xi_2 x-\omega_2 t)} = e^{i\xi_2 x}e^{-i(\xi_2^2-c_2)t},\\ \psi_3(x,t) &= e^{i(\xi_3 x-\omega_3 t)} = e^{i\xi_3 x}e^{-i(\xi_3^2-c_1)t}. \end{aligned} \tag{5.10}$$

Notice that the dispersion relations (5.9) are real and the plane waves (5.10) propagate with the phase velocities ω_1/ξ_1, ω_2/ξ_2, ω_3/ξ_3, respectively, with no decay in amplitude. This shows that the equation (5.6) under consideration is dissipative. The group velocities are

$$\frac{d\omega_1}{d\xi_1} = 2\xi_1, \quad \frac{d\omega_2}{d\xi_2} = 2\xi_2, \quad \frac{d\omega_3}{d\xi_3} = 2\xi_3, \tag{5.11}$$

which describe the velocities of different waves. The group velocity dispersions

$$\frac{d^2\omega_1}{d\xi_1^2} = 2, \quad \frac{d^2\omega_2}{d\xi_2^2} = 2, \quad \frac{d^2\omega_3}{d\xi_3^2} = 2 \tag{5.12}$$

are nonzero and independent of the wave number. So, waves with different wave number travel with the same velocities. Therefore, spatial separation of wave packets are not expected.

5.2 Numerical Dispersion Relation

In this section we will consider the discrete plane wave of the linear 3−CNLS equation (5.6) corresponding to the plane wave solution (5.7). We notice that, the linear equations (5.6) are uncoupled equations and differs only by constants c_1 and c_2. We also notice that, the dispersion relations (5.9) are all parabolic equations in terms of the frequency and all differ by constants c_1 and c_2. For this reason, we will find numeric dispersion relation only for the first equation

$$i\psi_{1t} + \psi_{1xx} + c_1\psi_1 = 0 \tag{5.13}$$

in (5.6), for simplicity. The numeric dispersion relations for the other equations in (5.6) can be obtained similarly. We will consider the discrete plane wave

$$\overline{\psi_1}_j^n = \hat{u}e^{i(\xi_1 x_j - \omega_1 t_n)} = \hat{u}e^{i(j\xi_1\Delta x - n\omega_1\Delta t)}, \quad i = \sqrt{-1} \tag{5.14}$$

which is the discrete version of the Fourier mode (5.4). As in the continuous plane wave solutions (5.10), each mode is a solution of the numerical method if the wave number ξ_1 and the frequency ω_1 satisfy the numeric dispersion relation. In order to obtain the dissipation and dispersion information for all finite Fourier transform solutions of a finite difference method, we consider the terms $\xi_1\Delta x$ and $\omega_1\Delta t$ in the ranges $-\pi \leq \xi_1\Delta x \leq \pi$ and $\pi \leq \omega_1\Delta t \leq \pi$ ([70]).

In order to obtain the numeric dispersion relation of the AVF scheme, we apply the AVF method to the linear equation (5.13),

$$\begin{aligned} i\frac{\psi_1{}_j^{n+1} - \psi_1{}_j^n}{\Delta t} = \frac{-1}{\Delta x^2}\int_0^1 \Big[(1-\xi)\left(\psi_1{}_{j-1}^{n+1} - 2\psi_1{}_j^{n+1} + \psi_1{}_{j+1}^{n+1}\right) + \xi\left(\psi_1{}_{j-1}^{n} - 2\psi_1{}_j^{n} + \psi_1{}_{j+1}^{n}\right) \\ -c_1\left((1-\xi)\psi_1{}_j^{n+1} + \xi\psi_1{}_j^n\right)\Big]\,d\xi. \end{aligned} \tag{5.15}$$

Substituting the discrete plane wave (5.14) into (5.15) and the taking the integral, we get

$$\begin{aligned} i\hat{u}\left(e^{i(j\xi_1\Delta x-(n+1)\omega_1\Delta t)} - e^{i(j\xi_1\Delta x - n\omega_1\Delta t)}\right) = \\ \frac{-\hat{u}\Delta t}{2\Delta x^2}\Big(e^{i((j-1)\xi_1\Delta x-(n+1)\omega_1\Delta t)} - 2e^{i(j\xi_1\Delta x-(n+1)\omega_1\Delta t)} + e^{i((j+1)\xi_1\Delta x-(n+1)\omega_1\Delta t)} \\ +e^{i((j-1)\xi_1\Delta x-n\omega_1\Delta t)} - 2e^{i(j\xi_1\Delta x-n\omega_1\Delta t)} - e^{i((j+1)\xi_1\Delta x-n\omega_1\Delta t)}\Big) \\ -\frac{c_1\Delta t}{2}\hat{u}\left(e^{i(j\xi_1\Delta x-(n+1)\omega_1\Delta t)} + e^{i(j\xi_1\Delta x-n\omega_1\Delta t)}\right). \end{aligned} \tag{5.16}$$

Dividing both side of (5.16) by $\hat{u}e^{i(j\xi_1\Delta x - n\omega_1\Delta t)}$ yields

$$i(e^{-i\omega_1\Delta t} - 1) = \frac{-\Delta t}{2\Delta x^2}\left(-4\sin^2(\frac{\xi_1\Delta x}{2})\right)(1 + e^{-i\omega_1\Delta t}) - \frac{c_1\Delta t}{2}(1 + e^{-i\omega_1\Delta t})$$

or we get

$$i\frac{(e^{-i\omega_1\Delta t} - 1)}{(e^{-i\omega_1\Delta t} + 1)} = \frac{\Delta t}{\Delta x^2}\left(2\sin^2(\frac{\xi_1\Delta x}{2})\right) - \frac{c_1\Delta t}{2}.$$

Using the identity

$$\frac{e^{i\theta} - e^{-i\theta}}{e^{i\theta} + e^{-i\theta}} = i\tan\theta$$

we obtain

$$i\left(-i\tan\frac{(\omega_1\Delta t}{2})\right) = \frac{\Delta t}{\Delta x^2}\left(2\sin^2(\frac{\xi_1\Delta x}{2})\right) - \frac{c_1\Delta t}{2}. \tag{5.17}$$

Therefore, we get

$$\tan\frac{\omega_1\Delta t}{2} = \frac{\Delta t}{\Delta x^2}\left(2\sin^2(\frac{\xi_1\Delta x}{2})\right) - \frac{c_1\Delta t}{2}. \tag{5.18}$$

Since $-\pi \leq \omega_1 \Delta t \leq \pi$ and tangent function is invertible on $(-\pi/2, \pi/2)$ we can write the frequency as

$$D_{1AVF}(\omega_1, \xi_1) := \omega_1 - \frac{2}{\Delta t} \arctan\left(\frac{\Delta t}{\Delta x^2}\left(2\sin^2(\frac{\xi_1 \Delta x}{2})\right) - \frac{c_1 \Delta t}{2}\right) = 0, \tag{5.19}$$

which is the numerical dispersion relation for the AVF method (5.15) of the 3–CNLS equation. Note that the equation (5.18) can be re-written as

$$\frac{\tan\frac{\omega_1 \Delta t}{2}}{\Delta t} = \frac{1}{\Delta x^2}\left(2\sin^2(\frac{\xi_1 \Delta x}{2})\right) - \frac{c_1}{2}. \tag{5.20}$$

which approaches to the continuous dispersion relation

$$\omega_1 = \xi_1^2 - c_1$$

when $(\Delta x, \Delta t) \to (0, 0)$, as given in (5.9). Following the same steps for the equations

$$\begin{aligned} i\psi_{2t} + \psi_{2xx} + c_2\psi_2 &= 0, \\ i\psi_{3t} + \psi_{3xx} + c_1\psi_3 &= 0. \end{aligned} \tag{5.21}$$

in the equation (5.6), one can obtain the numeric dispersion relations

$$\begin{aligned} D_{2AVF}(\omega_2, \xi_2) &:= \omega_2 - \frac{2}{\Delta t} \arctan\left(\frac{\Delta t}{\Delta x^2}\left(2\sin^2(\frac{\xi_2 \Delta x}{2})\right) - \frac{c_2 \Delta t}{2}\right) = 0, \\ D_{3AVF}(\omega_3, \xi_3) &:= \omega_3 - \frac{2}{\Delta t} \arctan\left(\frac{\Delta t}{\Delta x^2}\left(2\sin^2(\frac{\xi_3 \Delta x}{2})\right) - \frac{c_1 \Delta t}{2}\right) = 0. \end{aligned} \tag{5.22}$$

The numerical group velocity of the AVF method is given by

$$\frac{d\omega_{kAVF}}{d\xi_k} = \frac{2}{\Delta t}\left(1 + \left(\frac{\omega_k \Delta t}{2}\right)^2\right)\left(\frac{\Delta t}{\Delta x}\sin(\xi_k \Delta x)\right) \quad k = 1, 2, 3. \tag{5.23}$$

Now, we will obtain the numeric dispersion relation of the two–step method (3.28). Application of the two–step method (3.28) to the equation (5.13) yields

$$i\frac{{\psi_1}_j^{n+1} - {\psi_1}_j^{n-1}}{2\Delta t} + \delta_x^2\left(\frac{{\psi_1}_j^{n+1} + {\psi_1}_j^{n-1}}{2}\right) + c_1\left(\frac{{\psi_1}_j^{n+1} + {\psi_1}_j^{n-1}}{2}\right) = 0, \tag{5.24}$$

where

$$\delta_x^2 {\psi_1}_j^n = \frac{1}{\Delta x^2}\left({\psi_1}_{j-1}^n - 2{\psi_1}_j^n + {\psi_1}_{j+1}^n\right).$$

Substituting the discrete plane wave (5.14) into (5.24) we get

$$\begin{aligned} & i\bar{u}\left(\frac{e^{i(j\xi_1\Delta x-(n+1)\omega_1\Delta t)} - e^{i(j\xi_1\Delta x-(n-1)\omega_1\Delta t)}}{2\Delta t}\right) \\ & = \frac{-\bar{u}}{2\Delta x^2}\left(e^{i((j-1)\xi_1\Delta x-(n+1)\omega_1\Delta t)} - 2e^{i(j\xi_1\Delta x-(n+1)\omega_1\Delta t)} + e^{i((j+1)\xi_1\Delta x-(n+1)\omega_1\Delta t)}\right. \\ & \quad \left. +e^{i((j-1)\xi_1\Delta x-(n-1)\omega_1\Delta t)} - 2e^{i(j\xi_1\Delta x-(n-1)\omega_1\Delta t)} - e^{i((j+1)\xi_1\Delta x-(n-1)\omega_1\Delta t)}\right) \\ & \quad - \frac{c_1}{2}\bar{u}\left(e^{i(j\xi_1\Delta x-(n+1)\omega_1\Delta t)} + e^{i(j\xi_1\Delta x-(n-1)\omega_1\Delta t)}\right). \end{aligned} \tag{5.25}$$

Dividing both side of (5.25) by $\bar{u}e^{i(j\xi_1\Delta x - n\omega_1\Delta t)}$ yields

$$i\left(\frac{e^{-i\omega_1\Delta t} - e^{i\omega_1\Delta t}}{2\Delta t}\right) = -\frac{1}{\Delta x^2}\left(\frac{e^{-i\omega_1\Delta t} + e^{i\omega_1\Delta t}}{2}\right)\left(e^{i\xi_1\Delta x} + e^{-i\xi_1\Delta x} - 2\right) - c_1\left(\frac{e^{-i\omega_1\Delta t} + e^{i\omega_1\Delta t}}{2}\right),$$

which is equivalent to

$$\frac{\sin(\omega_1\Delta t)}{\Delta t} = \frac{-1}{\Delta x^2}\cos(\omega_1\Delta t)\left(-4\sin^2(\frac{\xi_1\Delta x}{2})\right) - c_1\cos(\omega_1\Delta t).$$

Since $-\pi \leq \omega_1\Delta t \leq \pi$ and $\cos(\omega_1\Delta t) \neq 0$, we multiply both sides by $1/\cos(\omega_1\Delta t)$ and get

$$\frac{\sin(\omega_1\Delta t)}{\Delta t\cos(\omega_1\Delta t)} = \frac{1}{\Delta x^2}\left(4\sin^2(\frac{\xi_1\Delta x}{2})\right) - c_1$$

or

$$\frac{\tan(\omega_1\Delta t)}{\Delta t} = \frac{1}{\Delta x^2}\left(4\sin^2(\frac{\xi_1\Delta x}{2})\right) - c_1. \tag{5.26}$$

We note that as $(\Delta x, \Delta t) \to (0, 0)$, the equation (5.26) approaches to the continuous dispersion relation

$$\omega_1 = \xi_1^2 - c_1$$

given in (5.9). Since $-\pi \leq \omega_1\Delta t \leq \pi$ and tangent function is invertible on $(-\pi/2, \pi/2)$ we can write the frequency as

$$D_{1TSM}(\omega_1, \xi_1) := \omega_1 - \frac{1}{\Delta t}\arctan\left(\frac{4\Delta t}{\Delta x^2}\sin^2(\frac{\xi_1\Delta x}{2}) - c_1\Delta t\right) = 0. \tag{5.27}$$

Following the same steps for the equations

$$\begin{aligned} i\psi_{2t} + \psi_{2xx} + c_2\psi_2 &= 0, \\ i\psi_{3t} + \psi_{3xx} + c_1\psi_3 &= 0 \end{aligned} \tag{5.28}$$

in the equation (5.6), one can obtain the numeric dispersion relations

$$\begin{aligned} D_{2TSM}(\omega_2, \xi_2) &:= \omega_2 - \frac{1}{\Delta t}\arctan\left(\frac{4\Delta t}{\Delta x^2}\sin^2(\frac{\xi_2\Delta x}{2}) - c_2\Delta t\right) = 0, \\ D_{3TSM}(\omega_3, \xi_3) &:= \omega_3 - \frac{1}{\Delta t}\arctan\left(\frac{4\Delta t}{\Delta x^2}\sin^2(\frac{\xi_3\Delta x}{2}) - c_1\Delta t\right) = 0. \end{aligned} \tag{5.29}$$

The numerical group velocity of the TSM method is given by

$$\frac{d\omega_{kTSM}}{d\xi_k} = \frac{1}{\Delta t}\left(1 + (\omega_k\Delta t)^2\right)\left(\frac{2\Delta t}{\Delta x}\sin(\xi_k\Delta x)\right), k = 1, 2, 3. \tag{5.30}$$

Figure 5.2 represents graph of continuous dispersion relation ω_1 in (5.9), numeric dispersion relation (5.19) of the AVF method and the numeric dispersion relation (5.27) for $\Delta x = 0.5$, $\Delta t = 0.1$ with $c_1 = 1$. For different c_1 values we have obtained similar pictures. When we compare the continuous dispersion relations (5.9) with the numeric dispersion relations of the AVF scheme (5.20), (5.22) and the numeric dispersion relation of the two–step scheme (5.26), (5.29), we see that the AVF method and the two–step method preserves the form of the continuous dispersion relations. Thus, we have proven the following:

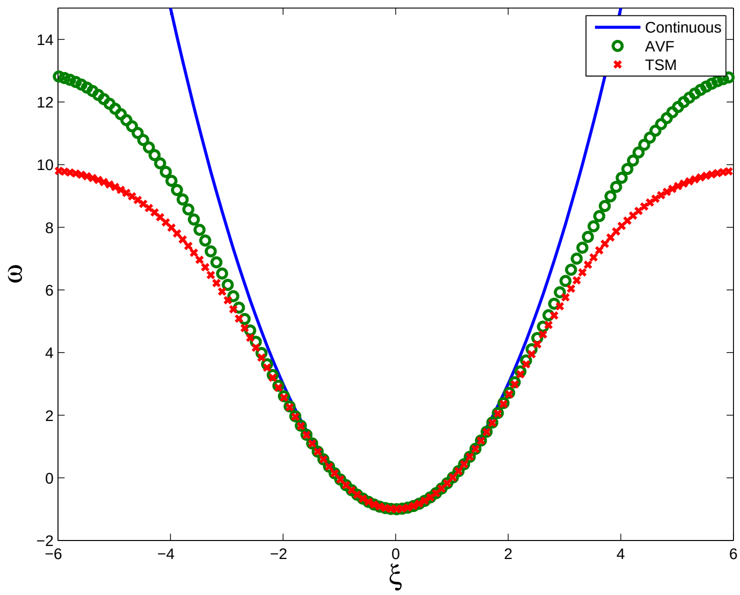


Figure 5.2: Continuous and numeric dispersion curves for ψ_1 of the linear system (2.2).

Proposition 5.2.1 *The energy preserving AVF scheme (3.11) and the mass conserving two–step method (3.28) (TSM) qualitatively preserves the dispersion relation of the linear* 3−*CNLS equation (5.6). Specifically, there exist diffeomorphism Z_1 and Z_2 satisfying the exact dispersion relation*

$$\begin{aligned}
D_{1AVF}(\omega_1,\xi_1) &= D_{1AVF}(Z_1(\omega_1),Z_2(\xi_1)) = Z_1 - Z_2^2 + c_1,\\
D_{2AVF}(\omega_2,\xi_2) &= D_{2AVF}(Z_1(\omega_1),Z_2(\xi_2)) = Z_1 - Z_2^2 + c_2,\\
D_{3AVF}(\omega_3,\xi_3) &= D_{3AVF}(Z_1(\omega_3),Z_2(\xi_3)) = Z_1 - Z_2^2 + c_1,\\
D_{1TSM}(\omega_1,\xi_1) &= D_{1TSM}(Z_1(\omega_1),Z_2(\xi_1)) = Z_1 - Z_2^2 + c_1,\\
D_{2TSM}(\omega_2,\xi_2) &= D_{2TSM}(Z_1(\omega_1),Z_2(\xi_2)) = Z_1 - Z_2^2 + c_2,\\
D_{3TSM}(\omega_3,\xi_3) &= D_{3TSM}(Z_1(\omega_3),Z_2(\xi_3)) = Z_1 - Z_2^2 + c_1,
\end{aligned} \tag{5.31}$$

where

$$\begin{aligned}
AVF:\quad (Z_1(\omega_k),Z_2(\xi_k)) &= \left(\frac{2\tan\left(\frac{\omega_k\Delta t}{2}\right)}{\Delta t},\frac{2\sin\left(\frac{\xi_k\Delta x}{2}\right)}{\Delta x}\right),\\
TSM:\quad (Z_1(\omega_k),Z_2(\xi_k)) &= \left(\frac{\tan\left(\frac{\omega_k\Delta t}{2}\right)}{\Delta t},\frac{2\sin\left(\frac{\xi_k\Delta x}{2}\right)}{\Delta x}\right),\quad k=1,2,3
\end{aligned} \tag{5.32}$$

for $-\pi \le \xi \le \pi$ and $-\pi \le \omega \le \pi$.

Diffeomorphism can be found for other equations and numerical methods such as multisyplectic integrators for NLS equation [73] and complex modified Korteweg–de Vries equation [74]. Shape preservation of the dispersion relations can also be seen from the graph of dispersion relations in Figure 5.2. From the figure we see that numeric dispersion relations of the AVF scheme and the two–step method (TSM) well preserves the continuous dispersion relation for small wave numbers

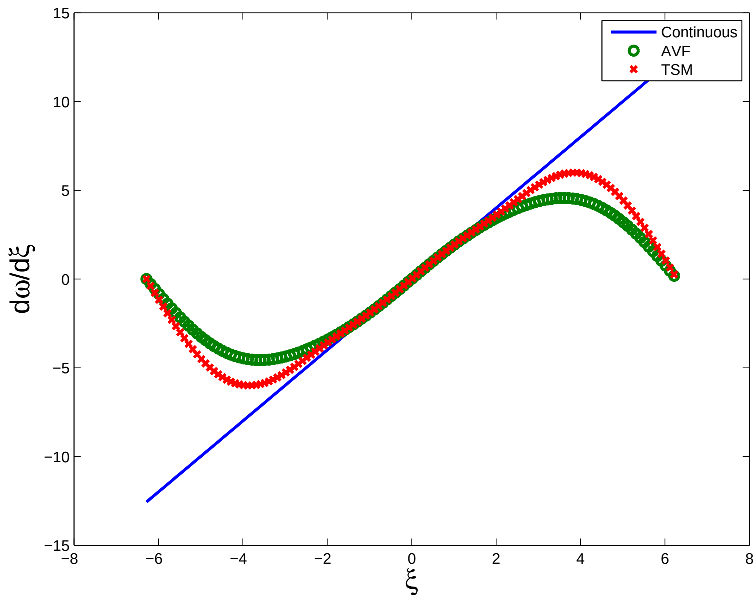


Figure 5.3: Group velocity curves for AVF and two–step method

(i.e. small ξ) which corresponds to long wave in plane wave solutions. On the other hand, for large wave numbers (i.e. short waves) the AVF method preserves the continuous dispersion relation better than the two-step method. There is no computational modes for each method because for every wave number there is only one frequency. In the following section we will verify these facts. Figure 5.3 represents the group velocity curves (5.11), (5.23) and (5.30). From the figure we see that sign of the group velocity is preserved for long waves (i.e. small ξ), but not preserved for the short waves (i.e. large ξ) for the AVF method and two–step method. This means that for high frequency waves, numeric plane waves and exact plane waves may move to different directions. In addition, we see that the group velocity curve of the two–step method is above the group velocity curve of AVF method for $0 \leq \xi \leq 2\pi$. This shows that some numerical modes of the two–step method travel faster than the numerical modes of the AVF method.

5.3 Plane Wave Solution

In this section, we consider the exact plane wave solution for the 3-CNLSE (2.2) with initial conditions given in (2.3) and periodic boundary conditions given in (2.4). We choose $\alpha_1 = \alpha_2 = \alpha_3 = 1$ and $\sigma = e = 2\mu$. Then the plane wave solution is

$$\psi_k(x,t) = A_k e^{i\left(\frac{\xi_k \pi x}{r} - \omega_k t\right)}, \qquad k = 1, 2, 3. \tag{5.33}$$

where

$$\omega_k = \frac{\xi_k^2 \pi^2}{r^2} - 2\mu \sum_{p=1}^{3} \left|A_p\right|^2, \qquad k = 1, 2, 3. \tag{5.34}$$

$r = (x_R - x_L)/2$, and A_k, ξ_k are constants. For numerical simulation the discrete analog of the plane wave solution (5.33) is [71]

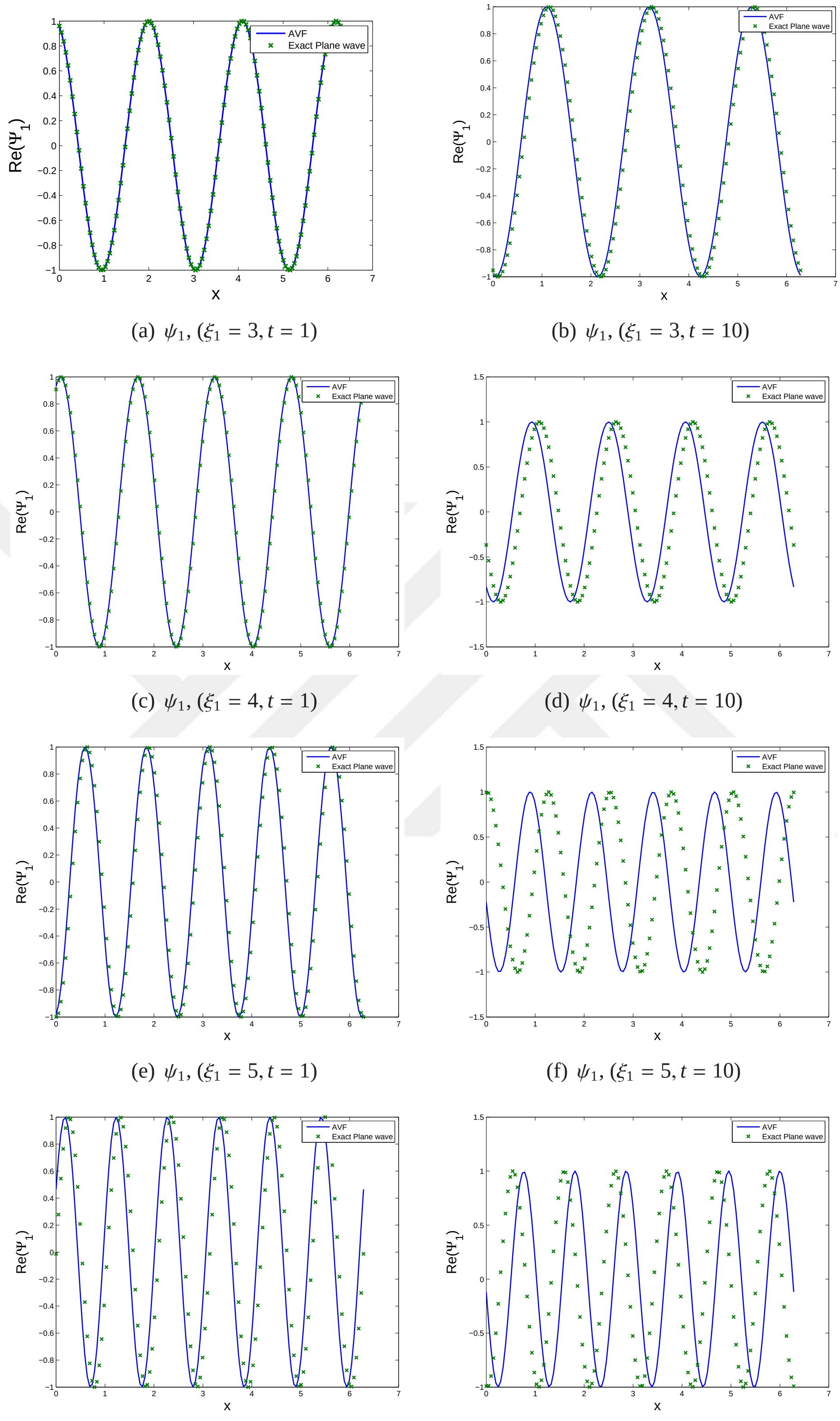
$$\psi_{k,j}^n(x,t) = A_k e^{i\left(\frac{\xi_k \pi j \Delta x}{r} - \omega_k n \Delta t\right)}, \qquad j = 0, 1, \cdots, M, \qquad k = 1, 2, 3. \tag{5.35}$$

5.3.1 Numerical Experiments

We consider the system (2.2) with the initial conditions (2.3) and the periodic boundary conditions (2.4) by using the AVF method (3.11) and the two–step method (3.28). The problem is solved in the region $x \in [0, 2\pi]$ and $T \in [0, 10]$ with $M = 128$ and $\Delta t = 0.01$. We choose $r = (2\pi - 0)/2$, $\mu = 0.5$ and the amplitudes $A_1 = A_2 = A_3 = 1$ in (5.35). Then the plane wave solution for the 3-CNLS equation (2.2) can be written as

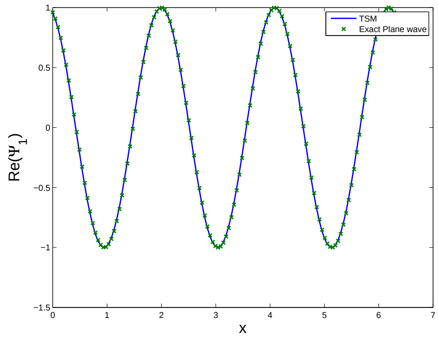
$$\psi_{k,\xi_k} = \exp\left[i(\xi_k x - \omega_k t)\right], \tag{5.36}$$

where $\omega_k = \xi_k^2 - 3$ is calculated from (5.34). Figures 5.4 and 5.5 represent the evolution of the plane wave solution for the AVF scheme (3.11) and the two–step scheme (3.28) with the exact plane wave solution (5.33). The figures show the behavior of the plane wave solution at different time levels $t = 1$ and $t = 10$ for different wave numbers such as $\xi_k = 3, \xi_k = 4, \xi_k = 5, \xi_k = 6$, $k = 1, 2, 3$. It is known that small values of ξ_k corresponds to low–frequency waves (or long wave) and the large values of ξ_k corresponds to the high–frequency waves (or short waves). In each figure in Figure 5.4 and Figure 5.5, we represent the real part of the wave $\psi_1(x,t)$ only since the solutions for $\psi_2(x,t)$ and $\psi_3(x,t)$ are similar to that of $\psi_1(x,t)$. From the figures we see that, for low–frequency waves the numerical solutions agree with the exact plane wave solution at $t = 1$. Note that, while the plane wave solution of the AVF method (3.11) still matches the exact one for $\xi_k = 5$, the plane wave solution of the two-step method (3.28) moves away from the exact one for $\xi_k = 5$. When the wave number increase to $\xi = 6$, we see that numerical solutions do not match the exact plane wave solution even at $t = 1$. In addition, numerical solutions moves away from the exact plane wave solution at time $t = 10$. When we compare the Figure 5.4(e) with the Figure 5.5(g), we see that the plane wave solution of the AVF method coincides with the exact plane wave solution better than the plane wave solution of the two–step method. This can be explained by the numeric and continuous dispersion relation. When we look at dispersion relation figures in Figure 5.2, we see that the dispersion relation of the AVF scheme is closer to the exact dispersion relation than that of the two-step scheme. That is why the plane wave solution of the AVF method (3.11) coincides with the exact one better than the two–step method (3.28) when the low–frequency waves are considered.

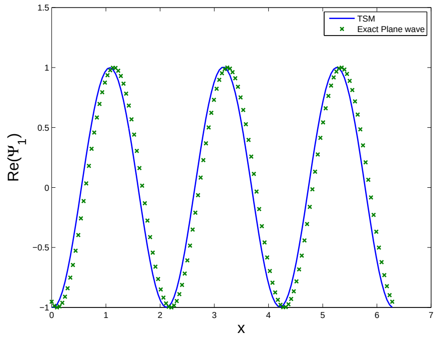


(a) $\psi_1, (\xi_1 = 3, t = 1)$
(b) $\psi_1, (\xi_1 = 3, t = 10)$
(c) $\psi_1, (\xi_1 = 4, t = 1)$
(d) $\psi_1, (\xi_1 = 4, t = 10)$
(e) $\psi_1, (\xi_1 = 5, t = 1)$
(f) $\psi_1, (\xi_1 = 5, t = 10)$
(g) $\psi_1, (\xi_1 = 6, t = 1)$
(h) $\psi_1, (\xi_1 = 6, t = 10)$

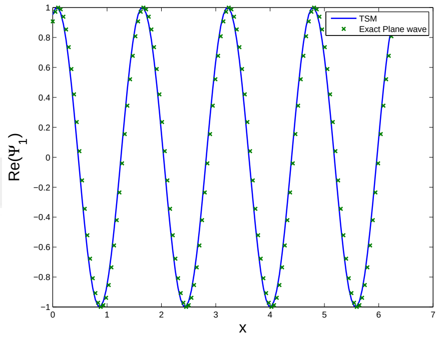
Figure 5.4: Plane wave solution: Reel part of $\psi_{k,\xi_k}(x, t)$ to system (2.2) with AVF method.



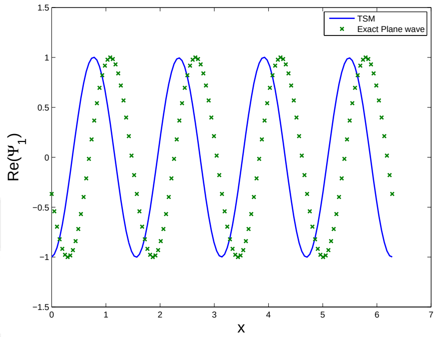
(a) $\psi_1, (\xi_1 = 3, t = 1)$



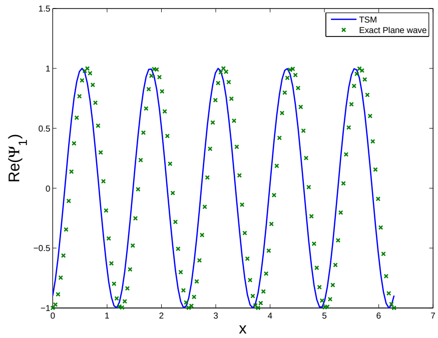
(b) $\psi_1, (\xi_1 = 3, t = 10)$



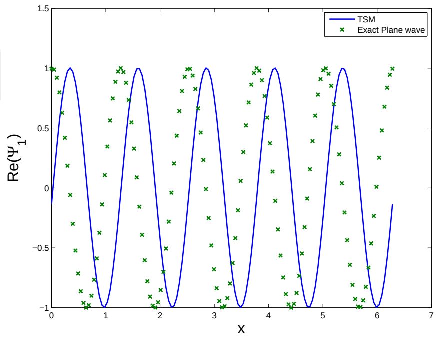
(c) $\psi_1, (\xi_1 = 4, t = 1)$



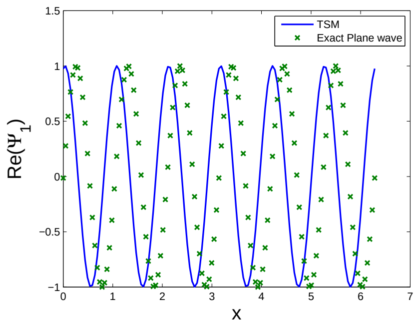
(d) $\psi_1, (\xi_1 = 4, t = 10)$



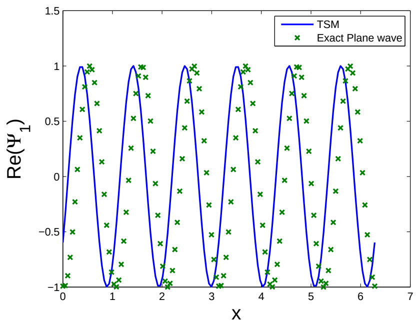
(e) $\psi_1, (\xi_1 = 5, t = 1)$



(f) $\psi_1, (\xi_1 = 5, t = 10)$



(g) $\psi_1, (\xi_1 = 6, t = 1)$



(h) $\psi_1, (\xi_1 = 6, t = 10)$

Figure 5.5: Plane wave solution: Reel part of $\psi_{k,\xi_k}(x, t)$ to system (2.2) with two–step scheme.

CHAPTER 6

CONCLUSION

The N–coupled nonlinear Schrödinger equation is an important model that has been applied in science and engineering. For $N = 1$ and $N = 2$ many works have been done on the study of soliton propagation, elastic collision and shape–changing collision. Recently, the analysis has been extended to the case of N–CNLS with $N \geq 3$. In this thesis we have considered N–CNLS equation with $N = 3$ for which theoretical and numerical works are comparatively rare. The exact solution of 3–CNLS equation does not exist. However, for some special set of parameters exact soliton solutions have been obtained analytically. For this reason, numerical studies are essential to understand the behavior of the solution of 3–CNLSE for arbitrary set of parameters. We have developed and proven three finite difference conservative methods which are the energy conserving AVF method, the mass conserving two–step method and both the mass and the energy conserving one step method for numerical solution of the 3–CNLS equations. These methods are not symplectic and different from Runge–Kutta (RK) method. We performed the simulation of periodic wave, elastic collision and interaction scenario of three solitons to watch the proposed methods for long time simulation by observing the mass and the energy conservation properties. From the numerical results, we see that the one–step method preserves the energy better than the AVF method and preserves the mass better than the two–step method. Dispersion relation analysis of the energy conserving method and the mass conserving method are analyzed. Long wave and short wave preservation of the AVF method and two–step method are discussed.

Linear stability, accuracy and the convergence of the methods are also discussed. It is shown that all methods are linearly unconditionally stable. Numerical results verify the theoretical results for the methods are conservative. In addition, numerical results show that all schemes well simulate the periodic wave, single soliton and the colliding soliton of the 3–CNLS equation. By changing the wave–wave interaction coefficient of the equation, different colliding scenarios such as creation of a new vector soliton and fusion of solitons are observed.

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