ENERGY PRESERVING METHODS FOR KORTEWEG DE VRIES TYPE EQUATIONS

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submitted by **GÖRKEM ŞİMŞEK** in partial fulfillment of the requirements for the degree of **Master of Science in Department of Scientific Computing, Middle East Technical University** by,

Prof. Dr. Ersan Akyıldız _____
Director, Graduate School of **Applied Mathematics**

Prof. Dr. Bülent Karasözen _____
Head of Department, **Scientific Computing**

Prof. Dr. Bülent Karasözen _____
Supervisor, **Department of Mathematics, METU**

Assist. Prof. Dr. Ayhan Aydın _____
Co-supervisor, **Department of Mathematics, Atılım University**

Examining Committee Members:

Prof. Dr. Tanıl Ergenç _____
Department of Mathematics, Atılım University

Prof. Dr. Bülent Karasözen _____
Department of Mathematics & Institute of Applied Mathematics, METU

Assist. Prof. Dr. Ayhan Aydın _____
Department of Mathematics, Atılım University

Assoc. Prof. Dr. Ömür Uğur _____
Institute of Applied Mathematics, METU

Assist. Prof. Dr. Ali Devin Sezer _____
Institute of Applied Mathematics, METU

Date: _____

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Name, Last Name: GÖRKEM ŞİMŞEK

Signature :

ABSTRACT

ENERGY PRESERVING METHODS FOR KORTEWEG DE VRIES TYPE EQUATIONS

Şimşek, Görkem
M.S., Department of Scientific Computing
Supervisor : Prof. Dr. Bülent Karasözen
Co-Supervisor : Assist. Prof. Dr. Ayhan Aydın

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Two well-known types of water waves are shallow water waves and the solitary waves. The former waves are those waves which have larger wavelength than the local water depth and the latter waves are used for the ones which retain their shape and speed after colliding with each other. The most well known of the latter waves are Korteweg de Vries (KdV) equations, which are widely used in many branches of physics and engineering. These equations are nonlinear long waves and mathematically represented by partial differential equations (PDEs). For solving the KdV and KdV-type equations, several numerical methods were developed in the recent years which preserve their geometric structure, i.e. the Hamiltonian form, symplecticity and the integrals. All these methods are classified as symplectic and multisymplectic integrators. They produce stable solutions in long term integration, but they do not preserve the Hamiltonian and the symplectic structure at the same time.

This thesis concerns the application of energy preserving average vector field integrator(AVF) to nonlinear Hamiltonian partial differential equations (PDEs) in canonical and non-canonical forms. Among the PDEs, Korteweg de Vries (KdV) equation, modified KdV equation, the Ito's system and the KdV-KdV systems are discetrized in space by preserving the skew-

symmetry of the Hamiltonian structure. The resulting ordinary differential equations (ODEs) are solved with the AVF method. Numerical examples confirm that the energy is preserved in long term integration and the other integrals are well preserved too. Soliton and traveling wave solutions for the KdV type equations are accurate as those solved by other methods. The preservation of the dispersive properties of the AVF method is also shown for each PDE.

Keywords: Korteweg de Vries equation, bi-Hamiltonian systems, energy preservation, dispersion, average vector field integrator

ÖZ

KORTEWEG DE VRIES TÜRÜNDEKİ DENKLEMLER İÇİN ENERJİYİ KORUYAN YÖNTEMLER

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Yüzeysel ve tek dalgalar en iyi bilinen iki su dalgası çeşididir. Yüzeysel dalgalar, dalgaboyu suyun yerel derinliğinden büyük olan dalgalardır. Tekli (soliton) dalgalar ise birbirleriyle çarpıştıktan sonra başlangıçtaki şekil ve hızlarını koruyanlardır. Fizik ve matematikte sık sık karşılaşılan tekli dalgaların çoğu Korteweg de Vries (KdV) şeklindeki denklemlerle doğrusal olmayan kısmi türevli denklem şeklinde ifade edilmektedir. Son yıllarda KdV denklemi ve benzer denklemlerin çözümü için Hamilton ve simplektik yapıları ile ilk integralleri gibi geometrik özelliklerini koruyan birçok sayısal yöntem geliştirilmiştir. Bu yöntemler simplektik ve çoklu-simplektik yöntemler olarak sınıflandırılmakta olup, bunlar uzun vadeli hesaplamalar sonucunda istikrarlı sonuçlar üretirken, denklemlerin Hamilton ve simplektik yapılarını aynı anda korumak mümkün olmamaktadır.

Bu tez ortalama vectör alan (OVA) yönteminin Hamilton yapıdaki doğrusal olmayan kısmi diferansiyel denklemlere uygulanması ile ilgilidir. Bu kısmi diferansiyel denklemlerden KdV denklemi, değiştirilmiş KdV denklemi, Ito sistemi ve KdV-KdV sistemleri Hamilton yapılarının aykırı simetrik özellikleri korunarak uzayda ayrıklaştırılmışlar ve elde edilen adi diferan-

siyel denklemler OVA yöntemi ile çözülmüştür. Uzun zamanlı integrasyon sonucunda denklemlerin enerjisinin ve diğer integrallerinin iyi korunduğu sayısal örneklerle doğrulanmıştır. Çözülen her denklem için OVA yönteminin dağılım özelliklerini ne ölçüde koruduğu gösterilmiştir.

Anahtar Kelimeler: Korteweg de Vries Denklemi, ikili Hamilton sistemler, enerji korunumu, dalga dağılımı, ortalama vektör alan yöntemi

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TABLE OF CONTENTS

LIST OF FIGURES

FIGURES

CHAPTER 1

INTRODUCTION

The subject of this thesis is the application of the energy preserving average vector field (AVF) integrators to Korteweg de Vries type equations in Hamiltonian and bi-Hamiltonian form and investigation of the dispersive properties of the discretized equation.

Traditionally, numerical integration of ordinary and partial differential equations concerns itself with the construction of numerical methods to minimize the global error, to ensure the numerical stability and to control the time step. In the last two decades, the concept of the design of numerical integrators shifted to preserve the intrinsic geometric properties, like to preserve the symplectic structure, symmetries, conserved quantities, the volume and phase space structure. These methods are known as geometric or structure preserving integrators. Most of the studies are concentrated in construction of symplectic and multisymplectic integrators for Hamiltonian ordinary and partial differential equations (See [28, 35, 51]). It is known that all Runge-Kutta methods preserve the linear integrals of the associated differential equations, and that only symplectic Runge-Kutta methods preserve the quadratic integrals. No Runge-Kutta method preserves higher order polynomial or nonlinear integrals. It was also shown that it is not possible to preserve symplectic structure and Hamiltonians simultaneously [51]. In addition to the fact that the integrators mentioned above fail to preserve many structure properties of the equations at the same time, there are also no methods except symplectic integrators constructed as general integrators to be applicable for canonical, non-canonical Hamiltonian or Poisson differential equations [33]. Recently, other type of integrators were investigated in the literature instantaneously, namely the so called energy or integral preserving integrators. Among the most well known is the AVF method developed for the canonical and non-canonical Hamiltonian systems [15, 27].

The outline of the thesis is as follows:

In Chapter 2 we outline the main properties of the Hamiltonian partial differential equations by emphasizing the bi-Hamiltonian structure and in Chapter 3 the chronological development of the AVF method is examined by comparing the properties of the method theoretically with other energy preserving methods. Chapter 4 is about the implementation of the AVF method for the Korteweg de Vries (KdV), modified KdV equations and the coupled system of equations like the Ito's system and the KdV-KdV system. The long term preservation of the energy (Hamiltonian) and the Casimir (integrals) are shown numerically and the soliton solutions are computed for each equation for different initial and boundary conditions in Chapter 5. Finally, Chapter 6 is an investigation of the dispersive properties of the AVF methods. The thesis ends with some conclusions.

CHAPTER 2

HAMILTONIAN and BI-HAMILTONIAN SYSTEMS

The Hamiltonian differential equations occur in many field such as ideal continuum mechanics, celestial mechanics, electrodynamics, quantization theory cosmology and nonlinear optics.

In this chapter, we will give the main properties of finite and infinite dimensional Hamiltonian systems. We will mainly focus on bi-Hamiltonian systems and some of them will be solved in the next chapters using average vector field method (AVF).

In the following sections, we make use of the material in [7, 33, 37] and Chapters 6, 7 in [46].

2.1 Basics of Finite-Dimensional Hamiltonian Systems

The finite and the infinite dimensional Hamiltonian systems are characterized by the so called Poisson bracket. The Poisson bracket maps the pair of smooth and real-valued functions F, G to a third function $\{F, G\}$, which are all defined on a smooth manifold $\mathcal{M}$.

Definition 2.1 *Let F, G and L are arbitrary smooth real-valued functions on $\mathcal{M}$. The* ***Poisson Bracket*** $\{\cdot, \cdot\}$ *satisfies four basic properties, which are*

- ***Bi-Linearity****:* $\{aF + bG, L\} = a\{F, L\} + b\{G, L\}, \quad \{F, aG + bL\} = a\{F, G\} + b\{F, L\}$, *where a, b are real constants.*
- ***Skew-Symmetry****:* $\{F, G\} = -\{G, F\}$,
- ***Leibniz' Rule****:* $\{F, G \cdot L\} = \{F, G\} \cdot L + G \cdot \{F, L\}$, *where $' \cdot '$ presents the ordinary multiplication of functions.*

- ***Jacobi Identity***: $\{\{F, G\}, L\} + \{\{L, F\}, G\} + \{\{G, L\}, F\} = 0.$

If the manifold $\mathcal{M}$ has a Poisson bracket, it is called a Poisson manifold and the bracket is said to define a Poisson structure on $\mathcal{M}$. The Poisson manifolds are a general case of symplectic manifolds, which arise in the Hamiltonian formulation of the classical mechanics. The symplectic manifolds are smooth manifolds and equipped with differential symplectic forms. The manifolds force symplectic forms to be non-degenerate, that is, symplectic forms has to be skew-symmetric. For these forms to be invertible, the symplectic manifolds should be even dimensional; the Poisson manifolds, on the other hand, can be determined on any Euclidean space with an arbitrary dimension.

Definition 2.2 *Let $\mathcal{M}$ be a Poisson manifold and $P : \mathcal{M} \to \mathbb{R}$ a real-valued, smooth function, which has the condition $\{P, H\} = 0$, for all functions H in $\mathcal{M}$. Then the function P is called a* ***distinguished*** *or* ***Casimir function***.

For an even dimensional manifold $\mathcal{M} = \mathbb{R}^m$, where $m = 2n$ and n is an integer, with coordinates $(p, q) = (p^1, \ldots, p^n, q^1, \ldots, q^n)$, a bracket can be defined as

$$\{F, G\} = \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q^i} \frac{\partial G}{\partial p^i} - \frac{\partial F}{\partial p^i} \frac{\partial G}{\partial q^i} \right) \tag{2.1}$$

with the identities

$$\{q^i, p^i\} = 1, \quad \{q^i, p^j\} = 0 \quad (\text{for} \quad i \neq j), \quad \{p^i, p^j\} = 0, \quad \{q^i, q^j\} = 0, \tag{2.2}$$

for $i, j = 1, \ldots, n$. This bracket satisfies the Definition 2.1 and it is called the canonical Poisson bracket which is widely used in classical mechanics. The only Casimir functions for canonical Poisson brackets are constants, that is, a function P satisfies

$$\{P, H\} = \sum_{i=1}^{n} \left(\frac{\partial P}{\partial q^i} \frac{\partial H}{\partial p^i} - \frac{\partial P}{\partial p^i} \frac{\partial H}{\partial q^i} \right) = 0, \text{ for all } H$$

if and only if it is constant.

In particular, if the Poisson bracket is defined as trivial, such that $\{F, G\} = 0$, for all $F, G \in \mathcal{M}$ then each function automatically becomes a Casimir function.

The Lie bracket plays an important role in the theory of Hamiltonian systems as well as the Poisson bracket.

Definition 2.3 *For a Poisson manifold $\mathcal{M}$ and a smooth function $H : \mathcal{M} \to \mathbb{R}$, the* ***Hamiltonian vector field*** *associated with H is defined as the unique smooth vector field with the property*

$$X_H(F) = \{F, H\} = -\{H, F\}.$$

To give an example of a Hamiltonian vector field, the canonical Poisson bracket of the manifold of dimension $m = 2n + l$ can be considered. Here, in addition to the coordinates p, q with the properties (2.2), r is also introduced as l dimensional and with the following extra relations

$$\{r^j, r^k\} = \{p^i, r^k\} = \{q^i, r^k\} = 0, \quad \text{for} \quad i = 1, \dots, n \quad \text{and} \quad j, k = 1, \dots, l.$$

Using (2.1) and the Definition 2.1 the Hamiltonian vector field is

$$X_H = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p^i} \frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p^i} \right).$$

The Hamiltonian equations control the flow of the Hamiltonian vector field and can be found integrating the following Hamilton's equations

$$\frac{dr^k}{dt} = 0, \quad \text{for} \quad k = 1, \dots, l, \tag{2.3}$$

$$\frac{dq^i}{dt} = \frac{\partial H}{\partial p^i}, \qquad \frac{dp^i}{dt} = -\frac{\partial H}{\partial q^i}, \quad \text{for} \quad i = 1, \dots, n. \tag{2.4}$$

The equations in (2.4) are the Hamilton's equations of Newtonian physics. Therefore, in classical mechanics the coordinate r becomes a Casimir function. In particular, if the Hamiltonian function H, that we are finding the vector field on, depends only on r, then the flow is zero. As a quick generalization of this fact, the Hamiltonian vector field of a specific function is zero everywhere if and only if this function is a Casimir function.

A general m-dimensional Poisson manifold $\mathcal{M}$ has the local coordinates $x = (x^1, \dots, x^m)$. Let $H(x)$ be a real-valued function and the related Hamiltonian vector field X_H defined as

$$X_H = \sum_{i=1}^{m} \xi^i(x) \frac{\partial}{\partial x^i}, \tag{2.5}$$

where $\xi^i(x)$ are H-dependent coefficient functions.To find the coefficient functions, using the Definition 2.1 we can write

$$X_H = \{\cdot, H\} = -\{H, \cdot\} = \sum_{i=1}^{m} \xi^i(x) \frac{\partial}{\partial x^i}$$

to get

$$X_H(x^c) = \{x^c, H\} = \xi^c(x), \quad \text{for any} \quad c \in \{1, \dots, m\}.$$

Therefore, the bracket is obtained as

$$\{F, H\} = \sum_{i=1}^{m} \{x^i, H\} \frac{\partial F}{\partial x^i}.$$

Using the skew-symmetry property of the Poisson bracket, a general definition with the real-valued functions F, G is introduced as

$$\{F, G\} = \sum_{i=1}^{m} \sum_{j=1}^{m} \{x^i, x^j\} \frac{\partial F}{\partial x^i} \frac{\partial G}{\partial x^j}. \tag{2.6}$$

After the definition of the general Poisson bracket, one can ask how to find the Poisson bracket of any two from of the set of the local coordinates. Let us call

$$J_{ij}(x) = \{x^i, x^j\}, \quad i, j = 1, \dots, m, \tag{2.7}$$

the *structure functions* and let each bracket corresponds to the $(i, j)th$ element of the $m \times m$ skew-symmetric *structure matrix*, $J(x)$. Hence (2.6) takes the form

$$\{F, H\} = \nabla F \cdot J \nabla H, \tag{2.8}$$

using the matrix $J(x)$ and rewriting the sum of the gradients of the functions F and H.

Proposition 2.4 ([46]) *$J(x) = (J_{ij}(x))$ is an $m \times m$ structure matrix for (2.8) if and only if it satisfies the properties that the Poisson bracket has, which are:*

(i) Bi-linearity, Leibniz' Rule,

(ii) Skew-symmetry, $J_{ij}(x) = -J_{ji}(x), \quad i, j = 1, \dots, m,$

(iii) Jacobi Identity,

$$\sum_{l=1}^{m} \left\{ J_{il} \frac{\partial}{\partial x^l} J_{jk} + J_{kl} \frac{\partial}{\partial x^l} J_{ij} + J_{jl} \frac{\partial}{\partial x^l} J_{ki} \right\} = 0 \quad i, j, k = 1, \dots, m, \, forall x \in \mathcal{M}. \tag{2.9}$$

Proof. The bi-linearity of the structure matrix $J(x)$ and satisfying the Leibniz' rule are related directly with the definition (2.8), since the Poisson bracket already satisfies these properties. For the skew-symmetry of the Poisson bracket

$$\{F, H\} = \nabla F \cdot J \nabla H = \nabla H \cdot (-J) \nabla F = -\{H, F\}$$

is satisfied whenever the matrix J has skew-symmetry. It is needed to show the equivalence of (2.9) to the Jacobi identity of the Poisson bracket. Note that, by (2.6) and (2.7)

$$\left\{\left\{x^i, x^j\right\}, x^k\right\} = \sum_{l=1}^{m} J_{lk} \frac{\partial}{\partial x^l} J_{ij},$$

which shows the equivalence of the Jacobi identity for coordinate functions x^i, x^j and x^k. (2.9) can also be shown for general functionals $F, G, H : \mathcal{M} \to \mathbb{R}$,

$$\begin{aligned} \{\{F, G\}, H\} &= \sum_{k,l=1}^{m} J_{lk} \frac{\partial}{\partial x^l} \left\{ \sum_{i,j=1}^{m} J_{ij} \frac{\partial F}{\partial x^i} \frac{\partial G}{\partial x^j} \right\} \frac{\partial H}{\partial x^k} \\ &= \sum_{i,j,k,l} \left\{ J_{lk} \frac{\partial J_{ij}}{\partial x^l} \frac{\partial F}{\partial x^i} \frac{\partial G}{\partial x^j} \frac{\partial H}{\partial x^k} \right. \\ &+ \left. J_{lk} J_{ij} \left(\frac{\partial^2 F}{\partial x^l \partial x^i} \frac{\partial G}{\partial x^j} \frac{\partial H}{\partial x^k} + \frac{\partial F}{\partial x^i} \frac{\partial^2 G}{\partial x^l \partial x^j} \frac{\partial H}{\partial x^k} \right) \right\}. \end{aligned}$$

Here, the second term cancels due to the skew-symmetry of the structure matrix and the first term is canceled by the virtue of (2.9). ■

Definition 2.5 *Let $x = (x^i, \ldots, x^m)$ be defined over an open subset $\mathcal{M} \subset \mathbb{R}^m$. Then a system of first order ordinary differential equation is a **Hamiltonian system** if $H(x)$ is a Hamiltonian function and $\mathrm{J}(x)$ is a structure matrix satisfying the Poisson bracket (2.1) and the system has the form of*

$$\frac{dx}{dt} = J(x) \nabla H(x) \tag{2.10}$$

or equivalently $\dot{x} = \{x, H\}$.

After the introduction of the finite-dimensional case, we can extend the definitions for the infinite dimensional Hamiltonian systems.

2.2 Infinite Dimensional Hamiltonian Systems

For Hamiltonian PDEs, the vector gradient operator ∇H has to be changed to the variational operator $\delta \mathcal{H}$ and the skew-symmetric matrix $J(x)$ becomes skew-adjoint matrix differential operator $\mathcal{J}(u)$.

The differential operator is defined as

$$\mathcal{P} = \int P \, dx \in \mathcal{F}.$$

With these conversions, the formulation of the Poisson bracket (2.6) becomes (2.11) for infinite dimensional systems.

$$\{\mathcal{P}, \mathcal{L}\} = \int \delta\mathcal{P} \cdot \mathcal{J} \cdot \delta\mathcal{L}\, dx, \quad \text{for functionals} \quad \mathcal{P}, \mathcal{L} \in \mathcal{F}. \tag{2.11}$$

The Poisson bracket with the functionals again satisfies the properties introduced in Definition 2.1. For the evolution equations, the result of the Poisson bracket of two functionals have to be a functional which is bi-linearly dependent on the variational derivatives of the initial functionals.

Even if the properties of the Poisson bracket are inherited from finite dimensional Hamiltonian systems, we need to define the differential operator $\mathcal{J}(u)$ for (2.11) to be a true Poisson bracket.

Definition 2.6 *Let $\mathcal{J}(u)$ be a linear operator. It is called Hamiltonian if the Poisson bracket (2.11) satisfies the properties of bi-linearity, skew-symmetry and the Jacobi identity as in the Definition 2.1.*

When the Poisson brackets are compared for the finite and the infinite dimensional systems, the bracket for the latter system does not need to satisfy the Leibniz' rule, since the rule in the finite dimension is used to show the existence of the Hamiltonian vector field of a real valued function $H(x)$, while it does not have any contribution to the bracket in the infinite dimensional case.

The Definition 2.2 gives clues about the determination of the Hamiltonian operator; however, it can be identified better using the following property.

Proposition 2.7 ([46]) *Let the bracket (2.11) be defined and let $\mathcal{J}(u)$ be a $q \times q$ differential operator. For the bracket to be skew-symmetric, $\mathcal{J}(u)$ has to be skew-adjoint, that is, $\mathcal{J}(u) = -\mathcal{J}^*(u)$ or $\mathcal{J}(u) + \mathcal{J}^*(u) = 0$, where $\mathcal{J}^*(u)$ stands for the Hermitian conjugate of $\mathcal{J}(u)$.*

Proof. Let $\mathcal{P}, \mathcal{L}$ be functionals such that $\mathcal{P} = \int P\, dx$ and $\mathcal{L} = \int L\, dx$, then by skew-symmetry property of the Poisson bracket

$$\int \delta\mathcal{P} \cdot \mathcal{J}(u) \cdot \delta\mathcal{L}\, dx = -\int \delta\mathcal{L} \cdot \mathcal{J}(u) \cdot \delta\mathcal{P}\, dx$$

and then

$$\int \delta\mathcal{P} \cdot (\mathcal{J}(u) + \mathcal{J}^*(u)) \cdot \delta\mathcal{L}\, dx = 0$$

if and only if $\mathcal{J}(u)$ is skew-adjoint. ■

The converse of the proposition also holds.

Corollary 2.8 *The differential operator $\mathcal{J}(u)$, which is a $q \times q$ skew-adjoint matrix, is a Hamiltonian operator when the matrix elements do not depend on u or its derivatives, that is the matrix is constant.*

After all these definitions and properties introduced, we can write the form of the Hamiltonian system of evolution equations as

$$\frac{\partial u}{\partial t} = \mathcal{J}(u)\ \frac{\delta \mathcal{H}}{\delta u}, \tag{2.12}$$

where $u(x,t) \in \mathbb{R}^q$, x is a p-tuple, $t \in \mathbb{R}$. The functionals $\mathcal{H}[u] = \int_\Omega H(x, u^n)\, dx$ is Hamiltonian functional with $\Omega \subset \mathbb{R}^p \times \mathbb{R}$ and $dx = dx_1\, dx_2 \ldots dx_p$ and $\mathcal{J}(u)$ is the Hamiltonian operator. Here, $\frac{\delta \mathcal{H}}{\delta u}$ represents the variational derivative of the Hamiltonian flow,which gives the answer of the question how the value of a functional $\mathcal{H}[u]$ changes with respect to a little change in $u(x)$, that is $u(x)$ is moved to $u(x) + \varepsilon\, \delta u(x)$, where the latter term is still in the domain Ω. The variational derivative can be investigated further with the functional calculus [44]. The first order change in $\mathcal{H}$ by δu is the first variation of the functional and can be written as

$$\begin{aligned} \delta\mathcal{H}[u;\delta u] &:= \lim_{\varepsilon\to 0} \frac{\mathcal{H}[u+\varepsilon\,\delta u] - \mathcal{H}[u]}{\Delta x} = \frac{d}{d\varepsilon}\mathcal{H}[u+\varepsilon\,\delta u]|_{\varepsilon=0} \\ &= \int_{x_0}^{x_1} \delta u\, \frac{\delta \mathcal{H}}{\delta u(x)}\, dx = \left\langle \frac{\delta \mathcal{H}}{\delta u}, \delta u \right\rangle, \end{aligned}$$

where $\frac{\delta \mathcal{H}}{\delta u}$ is the variational derivative of $\mathcal{H}$.

Now, let $\mathcal{H}[u] = \int_{x_0}^{x_1} H(x, u, u_x, u_{xx}, u_{xxx}, \ldots)\, dx$ be a general functional, the first variant becomes

$$\delta\mathcal{H}[u;\delta u] = \int_{x_0}^{x_1} \left(\frac{\partial H}{\partial u}\, \delta u + \frac{\partial H}{\partial u_x}\, \delta u_x + \frac{\partial H}{\partial u_{xx}}\, \delta u_{xx} + \ldots \right) dx,$$

applying integration by parts to the integral and canceling the boundary terms, which vanish due to the choice of δu, we result in the variational derivative

$$\frac{\delta \mathcal{H}}{\delta u} = \frac{\partial H}{\partial u} - \partial_x \left(\frac{\partial H}{\partial u_x} \right) + \partial_x^2 \left(\frac{\partial H}{\partial u_{xx}} \right) - \ldots$$

for a system such that $p = q = 1$.

A general variational derivative can be defined as

$$\frac{\delta \mathcal{H}}{\delta u_k} = \frac{\partial H}{\partial u_k} - \sum_{l=1}^{p} \frac{\partial}{\partial x_l}\left(\frac{\partial H}{\partial u_{k,l}}\right) + \dots \quad \text{for} \quad k = 1, \dots, q.$$

Likewise the finite dimensional case, there are distinguished functionals for evolution equations, which is because of the degeneracy of the Poisson bracket and leads to conservation laws for any system with Hamiltonian structure. Let us give the definition of the distinguished functionals for evolution equations this time.

Definition 2.9 *For a Hamiltonian differential operator $\mathcal{J}(u)$ of $q \times q$, the functional $C \in \mathcal{F}$ which satisfies the equation $\mathcal{J} \cdot \frac{\delta C}{\delta u} = 0$, for all x, u, is called the* ***distinguished functional****.*

As the vector field is defined by the Poisson bracket of two functionals with the Hamiltonian operator $\mathcal{J}$, the bracket is trivial for all $\mathcal{H} \in \mathcal{F}$ if and only if the functional C is distinguished. That means

$$\{\mathcal{H}, C\} = 0, \quad \text{for all} \quad \mathcal{H} \in \mathcal{F},$$

which tells that the corresponding Hamiltonian system of the functional C is $u_t = 0$ and this gives rise to conservation laws.

Proposition 2.10 *Let C be distinguished functional of a Hamiltonian operator $\mathcal{J}$, then every Hamiltonian system (2.12) relative to $\mathcal{J}$ has a conservation law that is determined by C.*

The distinguished functional determines a conservation law, but for the same Hamiltonian operator of the flow, there exists other conserved quantities within the concept of the symmetry group.

Definition 2.11 *Let (2.12) is the Hamiltonian field, then a scalar field $\mathcal{T}(u(t))$ is called a* ***conserved quantity****, if*

$$\frac{d}{dt}\mathcal{T}(u(t)) = \{\mathcal{H}, \mathcal{T}\} = 0.$$

With this definition, it can be also concluded that any distinguished functional is a conserved quantity automatically. Again using the Definition 2.2, one can easily show that the Poisson bracket of two time dependent conserved quantities results in another conserved quantity, that is

$$\frac{d}{dt}\{\mathcal{T}, \mathcal{V}\} = 0, \quad \text{where} \quad \mathcal{T}, \mathcal{V} \quad \text{are conserved quantities.}$$

For the Hamiltonian systems, there is another important concept of symmetry which is needed to determine all of the conserved quantities of the original equation.

Definition 2.12 *Let $u = f(x,t)$ be an arbitrary solution to a system and let G be a group of transformations such that for $g \in G$, $g \cdot f(x,t)$ is also a solution to the system. Then the group of G is called* ***symmetry group*** *of the given flow.*

For the following notions, let us use the Hamiltonian system as

$$\frac{\partial u}{\partial t} = K[u],$$

instead of (2.12).

Let the time dependent symmetry generator be $\sigma = \sigma(u,t)$ of the flow of the group transformations of G. Then σ satisfies the equation

$$\frac{\partial \sigma}{\partial t} + \{K, \sigma\} = 0.$$

In particular, if there is no time dependency for σ, then we have only the trivial Poisson bracket $\{K, \sigma\} = 0$.

For two different symmetries σ_1 and σ_2, the Poisson bracket $\{\sigma_1, \sigma_2\}$ gives again a symmetry, which is a trivial property of the group.

If the flow, that has the symmetry generator σ, is a Hamiltonian vector field, then we can write

$$\sigma = \mathcal{J} \cdot \frac{\delta \mathcal{I}}{\delta u}, \tag{2.13}$$

where $\mathcal{J}$ is the Hamiltonian operator and $\mathcal{I}$ is a conserved quantity. This notation gives clues about the relation between symmetries and the conserved quantities. The only thing to notice is that the equation (2.13) does not hold for all symmetries. That is, we can find symmetries which are not Hamiltonian.

Let us now explain the concept of symmetry, generators and the conserved quantities using the Korteweg de Vries (KdV) equation in an example.

Example: The general KdV equation has the form of

$$u_t = \alpha u u_x + \rho u_x + \nu u_{xxx}. \tag{2.14}$$

For simplicity, taking the constant values as $\alpha = 6$, $\rho = 0$ and $\nu = 1$, we obtain the following equation with the solution $u(x,t)$

$$u_t = 6uu_x + u_{xxx}. \tag{2.15}$$

To obtain the generators, we need some transformations, where the equation (2.15) is invariant. These transformations are space, time translations and Galilean, conformal transformations. Let now the new solution after transformations be $\bar{u}(\bar{x},\bar{t})$, which can be expressed in terms of the original solution $u(x,t)$ such that

- Space translation: $\bar{u}(\bar{x},\bar{t}) = u(x+\varepsilon,t)$,
- Time translation: $\bar{u}(\bar{x},\bar{t}) = u(x,t+\varepsilon)$,
- Galilean transformation: $\bar{u}(\bar{x},\bar{t}) = u(x+6\varepsilon t,t)+\varepsilon$,
- Conformal transformation: $\bar{u}(\bar{x},\bar{t}) = e^{2\varepsilon}u(e^{\varepsilon}x, e^{3\varepsilon}t)$.

Then the corresponding generators can be obtained as

$$\begin{aligned}
\sigma_1 &= u_x \approx \lim_{\varepsilon\to 0}\frac{u(x+\varepsilon,t)-u(x,t)}{\varepsilon},\\
\sigma_2 &= u_t \approx \lim_{\varepsilon\to 0}\frac{u(x,t+\varepsilon)-u(x,t)}{\varepsilon},\\
\sigma_3 &= 1+6tu_x \approx \lim_{\varepsilon\to 0}\frac{(u(x+6\varepsilon t,t)+\varepsilon)-u(x,t)}{\varepsilon},\\
\sigma_4 &= 2u+xu_x+3t(u_{xxx}+6uu_x) \approx \lim_{\varepsilon\to 0}\frac{e^{2\varepsilon}u(e^{\varepsilon}x,e^{3\varepsilon}t)-u(x,t)}{\varepsilon}.
\end{aligned}$$

Now using these symmetry generators, the conserved quantities can be found. For the well-known Hamiltonian operator $\mathcal{J}_1 = D$, the functional

$$\mathcal{I}_1 = \int u dx$$

is the trivial and independent Casimir functional, which gives the total mass physically.

As the first three generators can be written as in (2.13), one can easily check that the conserved quantities are

$$\mathcal{I}_2 = \int \frac{1}{2}u^2 dx, \quad \mathcal{I}_3 = \int \left(u^3 - \frac{1}{2}u_x^2\right)dx, \quad \mathcal{I}_4 = \int \left(xu+3tu^2\right)dx,$$

which agree with the first three generators for the equation

$$\sigma_i = \mathcal{J}_1 \cdot \frac{\delta \mathcal{I}_{i+1}}{\delta u}, \quad \text{for} \quad i = 1,2,3.$$

Since σ_4 can not be written in the form of (2.13), it does not construct a Hamiltonian vector field and does not give any conservation law.

2.2.1 Bi-Hamiltonian Systems

Definition 2.13 *Let $u_t = K_1[u]$ be a Hamiltonian system. It is called **bi-Hamiltonian** system, if it can be written in the form*

$$\frac{\partial u}{\partial t} = \mathcal{J}_1 \cdot \frac{\delta \mathcal{H}_2}{\delta u} = \mathcal{J}_2 \cdot \frac{\delta \mathcal{H}_1}{\delta u},$$

where $\mathcal{J}_1$ and $\mathcal{J}_2$ are Hamiltonian operators and $\mathcal{H}_1$ and $\mathcal{H}_2$ are appropriate Hamiltonian functionals.

Definition 2.14 *The Hamiltonian operators $\mathcal{J}_1$ and $\mathcal{J}_2$ are called **compatible** if every linear combination $a\mathcal{J}_1 + b\mathcal{J}_2$ is also a Hamiltonian operator for all $a, b \in \mathbb{R}$.*

Due to the compatibility condition of two operators, infinite symmetries and conservation laws for the system may be constructed recursively.

Let us start with a Casimir function $\mathcal{H}_0$ of the operator $\mathcal{J}_1$. Then using the symmetries between the Hamiltonian vector fields, a sequence of Hamiltonians is obtained. The following theorem gives the main idea and the recursion definition of the bi-Hamiltonian systems.

Theorem 2.15 ([46]) *Let $u_t = K_1[u] = \mathcal{J}_1 \cdot \frac{\delta \mathcal{H}_1}{\delta u} = \mathcal{J}_2 \cdot \frac{\delta \mathcal{H}_0}{\delta u}$ be a bi-Hamiltonian system of evolution equations and $\mathcal{R} = \mathcal{J}_2 \mathcal{J}_1^{-1}$ be the recursion operator to obtain Hamiltonian vector fields with $K_0[u] = \mathcal{J}_1 \cdot \frac{\delta \mathcal{H}_0}{\delta u}$. Now, let the vector fields defined recursively by*

$$K_n[u] = \mathcal{R} K_{n-1}[u], \quad \textit{for} \quad n \geq 1.$$

Then there exists an infinite sequence of $\mathcal{H}_0, \mathcal{H}_1, \mathcal{H}_2, \ldots$ such that each equation of the form

$$\mathcal{J}_1 \cdot \frac{\delta \mathcal{H}_n}{\delta u} = \mathcal{J}_2 \cdot \frac{\delta \mathcal{H}_{n-1}}{\delta u}, \quad \textit{with} \quad n \geq 1 \tag{2.16}$$

is a bi-Hamiltonian system.

Indeed, for each system (2.16), there exist infinite conservation laws with the property of the Hamiltonian functions $\mathcal{H}_n, \mathcal{H}_m$ such that

$$\{\mathcal{H}_n, \mathcal{H}_m\}_{\mathcal{J}_1} = \{\mathcal{H}_n, \mathcal{H}_m\}_{\mathcal{J}_2} = 0, \quad \textit{for} \quad n, m \geq 1$$

where the Poisson brackets are defined with respect to the first and the second Hamiltonian operators as

$$\{\mathcal{F},\mathcal{G}\}_{\mathcal{J}_1} = \int \frac{\delta \mathcal{F}}{\delta u}\mathcal{J}_1\frac{\delta \mathcal{G}}{\delta u}dx \quad \textit{and} \quad \{\mathcal{F},\mathcal{G}\}_{\mathcal{J}_2} = \int \frac{\delta \mathcal{F}}{\delta u}\mathcal{J}_2\frac{\delta \mathcal{G}}{\delta u}dx,$$

respectively.

In particular, for $l > k$ we have

$$\{\mathcal{H}_k,\mathcal{H}_l\}_{\mathcal{J}_1} = \{\mathcal{H}_{k-1},\mathcal{H}_l\}_{\mathcal{J}_2} = \{\mathcal{H}_{k-1},\mathcal{H}_{l+1}\}_{\mathcal{J}_1} = \ldots = \{\mathcal{H}_0,\mathcal{H}_{k+l}\}_{\mathcal{J}_1} = 0.$$

Example: There is a second operator $\mathcal{J}_2 = D^3 + 2(uD + Du)$ of the KdV equation (2.14) for which again the generators satisfy the equation

$$\sigma_i = \mathcal{J}_2 \cdot \frac{\delta \mathcal{I}_{i+1}}{\delta u},$$

for $i = 1, 2$ and 4. The conserved quantities are

$$\mathcal{I}_2 = \int \frac{1}{2}udx, \quad \mathcal{I}_3 = \int \frac{1}{2}u^2dx, \quad \mathcal{I}_5 = \int \left(\frac{1}{2}xu + \frac{3}{2}tu^2\right)dx,$$

whereas there is not any distinguished functional for the operator $\mathcal{J}_2$.

Now, with the second Hamiltonian formulation of the KdV equation, we obtained the conserved quantities with respect to both formulations. Now the recursion operator can be defined using the Theorem 2.2.1. Then the recursion operator of the KdV equation is

$$\mathcal{R} = \mathcal{J}_2\mathcal{J}_1^{-1} = \left[D^3 + 2(uD + Du)\right]D^{-1} = D^2 + 2u + 2DuD^{-1}.$$

According to the theorem, we can find infinitely many vector fields with the general recursion equation

$$u_{t_n} = R^nK_0 = \left[D^3 + 2(uD + Du)\right]^n u_x.$$

To obtain these vector fields, we need the first vector field $K_0[u]$, which can be derived by applying the recursion relation to the Lie symmetries [7], which results in $K_0[u] = u_x$. Then the following vector fields can be found recursively

$$K_1 = \mathcal{R}K_0 = \left(D^2 + 2u + 2DuD^{-1}\right)u_x = u_{xxx} + 6uu_x,$$
$$K_2 = \mathcal{R}^2K_0 = \mathcal{R}K_1 = \left(D^2 + 2u + 2DuD^{-1}\right)(u_{xxx} + 6uu_x) = u_{5x} + 13u_xu_{xx} + 5uu_{xxx} + 6u^2u_x,$$
$$\vdots$$

Then the corresponding conserved quantities are obtained as [46]

$$\begin{aligned}
\mathcal{H}_0 &= \int \frac{1}{2}u^2\,dx, \\
\mathcal{H}_1 &= \int \left(-\frac{1}{2}u_x^2 + u^3\right) dx, \\
\mathcal{H}_2 &= \int \left(\frac{1}{2}u_{xx}^2 + \frac{5}{2}u^2u_{xx} + \frac{5}{2}u^4\right) dx, \\
&\vdots
\end{aligned}$$

CHAPTER 3

ENERGY PRESERVING METHODS

In the last two decades the conservation of geometric properties of Hamiltonian differential equations in numerical integrators has attracted a lot of interest (see the monographs [23, 28, 35, 51]). Examples of such geometric properties are symplecticity, preservation of first integrals, symmetries, reversing symmetries and volume preservation. Runge-Kutta methods conserve linear invariants and only symplectic Runge-Kutta methods conserves quadratic invariants and symplecticity. Also, some Runge-Kutta methods are examined as pseudo symplectic methods, where the preservation of the energy in long time integration is tried [4]. No Runge-Kutta method conserves higher order polynomial or nonlinear invariants and the volume. It was also shown that it is not possible to preserve the symplecticness and Hamiltonian simultaneously [51]. Energy preserving methods are considered in the nineties as symplectic integrators and then they again gain attraction in recent years [20, 23, 30, 40, 42, 48]. The development of the energy preserving methods started with the work of Courant, Friedrichs and Lewy in 1928 [16]. New integrators are designed to preserve the first integrals for the differential equations using discrete gradients [41] and discrete variational derivative [20].

The energy preserving methods introduced first for the Hamiltonian ODEs with collocation methods [27] and improved as the average vector field method (AVF) [11] to apply the PDEs. It was shown in [12] that no Runge-Kutta method applied to Hamiltonian systems can be energy preserving.

The material in this Chapter is based on the articles [11, 15, 17, 27].

3.1 Energy Preserving Integrators

We consider the semidiscretized form of Hamiltonian PDEs (2.10)

$$\dot{u} = J(u)\nabla H(u) = f(u), \quad u \in \mathbb{R}^m, \tag{3.1}$$

where $J(u)$ is an antisymmetric matrix. An integral preserving method is constructed by introducing the discrete approximate gradient $\overline{\nabla} H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m$, which is a continuous mapping satisfying

$$\begin{aligned} H(u) - H(v) &= \overline{\nabla} H(v,u)^T (u - v), \\ \overline{\nabla} H(u,u) &= \nabla H(u). \end{aligned}$$

There exist several integral preserving methods in the literature satisfying the conditions above, but their construction is not unique. When the discrete gradient is found, the integral preserving method can be simply written as

$$\frac{u^{n+1} - u^n}{\Delta t} = \bar{J}(u^n, u^{n+1}) \overline{\nabla} H(u^n, u^{n+1}). \tag{3.2}$$

Examples of discrete gradient methods are proposed [23] as

$$\overline{\nabla} H(u,v) = \nabla H\left(\frac{v+u}{2}\right) + \frac{H(v) - H(u) - \nabla H\left(\frac{v+u}{2}\right)^T (v-u)}{\|v-u\|^2}(v-u)$$

and [29]

$$\overline{\nabla} H_{AVF} = \int_0^1 \nabla H((1-\tau)u^n + \tau u^{n+1})\, d\tau.$$

Then the Average Vector Field (AVF) method becomes with the choice of the second discrete gradient

$$\frac{u^{n+1} - u^n}{\Delta t} = J \overline{\nabla} H_{AVF} = J \int_0^1 \nabla H((1-\tau)u^n + \tau u^{n+1})\, d\tau \tag{3.3}$$

for canonical Hamiltonian systems.

To show the energy preservation of the AVF method, we multiply both sides with $\overline{\nabla} H_{AVF} = \int_0^1 \nabla H((1-\tau)u^n + \tau u^{n+1})\, d\tau$, which results in the equation

$$\overline{\nabla} H_{AVF}\, \frac{u^{n+1} - u^n}{\Delta t} = \overline{\nabla} H_{AVF}\, J\, \overline{\nabla} H_{AVF}. \tag{3.4}$$

As J is skew-symmetric, right hand side of (3.4) vanishes and one obtains

$$\overline{\nabla} H_{AVF} \frac{u^{n+1} - u^n}{\Delta t} = \int_0^1 \frac{u^{n+1} - u^n}{\Delta t} \nabla H((1-\tau)u^n + \tau u^{n+1})\, d\tau = 0,$$

which can be reduced to

$$\int_0^1 \frac{d}{d\tau}\left(H((1-\tau)u^n + \tau u^{n+1})\right) d\tau = 0.$$

By the fundamental theorem of calculus, we obtain

$$H(u^{n+1}) - H(u^n) = 0.$$

3.2 Average Vector Field Method

We will now give the AVF method for a general system of ODE's

$$\begin{aligned} u' &= f(u), \quad u \in \mathbb{R}^m, \\ u^{n+1} - u^n &= \Delta t \int_0^1 f\left((1-\tau)u^n + \tau u^{n+1}\right) d\tau. \end{aligned} \tag{3.5}$$

This method only requires the evaluation of the vector field. When applied to the Hamiltonian systems as in (3.3), it exactly preserves the energy of an arbitrary Hamiltonian. In addition, it is symmetric and it is a B-series method [13].

The AVF method is derived in [27] as an energy preserving collocation method. Let us given the Lagrange basis interpolation polynomials

$$l_i(\tau) = \prod_{j=1, j\neq i}^{s} \frac{\tau - c_j}{c_i - c_j}, \quad b_i = \int_0^1 l_i(\tau)\, d\tau. \tag{3.6}$$

Then the energy preserving collocation method is defined as

Definition 3.1 *Let $c_1, c_2, \ldots, c_s$ be distinct real numbers with the same property as in the original collocation methods such that $0 \leq c_i \leq 1$ and $b_i \neq 0$ for $1 \leq i \leq s$ and h is the time step. Now consider a polynomial $y(t)$ having degree s and satisfying*

$$\begin{aligned} y(t_0) &= u_0 \\ \dot{y}(t_0 + c_i h) &= \frac{1}{b_i} \int_0^1 l_i(\tau) f(y(t_0 + \tau h))\, d\tau. \end{aligned} \tag{3.7}$$

The next step is then defined by $u_1 = y(t_0 + h)$.

When the integrals are approximated by interpolating quadrature formulas, corresponding to the nodes $c_1, \ldots, c_s$, one obtains $\dot{y}(t_0 + c_i h) = f(y(t_0 + c_i h))$ and the method reduces to

the classical collocation method. Therefore, the method is named "the energy-preserving collocation method".

When $\dot{y}(t_0 + c_i h)$ is denoted as k_i and the methods can be summarized as

$$\dot{y}(t_0 + \tau h) = \sum_{i=1}^{s} l_i(\tau) k_i \tag{3.8}$$

$$y(t_0 + \tau h) = u_0 + h \sum_{i=1}^{s} \left(\int_0^{\tau} l_i(\xi)\, d\xi \right) k_i. \tag{3.9}$$

A nonlinear system of equations $k = G(k)$ for finite dimensional vector $k = (k_1, \ldots, k_s)$ is obtained when (3.9) is inserted into (3.7). This equation is solved by fixed point iteration or by Newton's method.

The integrals in (3.7) and (3.9) can be computed for polynomial Hamiltonians exactly at the beginning of the integration. For a non-polynomial Hamiltonian, the integrals have to be computed accurately by numerical quadrature formulas.

In polynomial Hamiltonians, the computational cost is comparable to the classical collocation methods like Gauss-Legendre Runge-Kutta methods [27].

The energy preserving collocation methods can be interpreted as continuous-stage Runge-Kutta methods [27] such that

$$K_\xi = u^n + \Delta t \int_0^1 a(\xi, \eta) f(K_\eta)\, d\eta, \quad u^{n+1} = u^n + \Delta t \int_0^1 b(\eta) f(K_\eta)\, d\eta, \tag{3.10}$$

for $\xi \in (0, 1)$. Here, $K_\xi \approx u(t_0 + c(\xi)\Delta t)$, where $c(\xi) = \int_0^1 a(\xi, \eta)\, d\eta$. The integral stages K_ξ correspond to the values of the polynomial $y(t_0 + \xi \Delta t)$ and the coefficients are given by

$$c(\xi) = \xi, \quad a(\xi, \eta) = \sum_{i=1}^{s} \frac{1}{b_i} \int_0^{\xi} l_i(\alpha)\, d\alpha\, l_i(\eta), \quad b(\eta) = 1. \tag{3.11}$$

The existence of the method (3.10) and other Runge-Kutta like methods such as AVF methods, the existence and the uniqueness of the solution can be ensured with the following theorem.

Theorem 3.2 ([13]) *Let the function $f : \mathbb{R}^n \to \mathbb{R}^n$ be continuous and satisfies the Lipschitz condition $|f(x_i) - f(x_j)| \leq K|x_i - x_j|$ for all $x_i, x_j \in \mathbb{R}^n$. If*

$$\Delta t < \frac{1}{K \sup_{\xi \in [0,1]} \int_0^1 |a(\xi, \eta)|\, d\eta},$$

then the solution (3.10) has a unique solution.

In particular, the AVF method always has a solution, this can be shown with the particular choice of the functions $a(\xi, \eta) = \xi$ and $b(\eta) = 1$.

The energy preserving collocation methods can be customized for $s = 1$ and $s = 2$ as in the following way:

- ***s = 1 :*** The method reduces to $y(t_0 + \tau h) = (1 - \tau)u_0 + \tau u_1$, which corresponds to the average vector field method. This consequence is independent of the choice of the constant c_1.
- ***s = 2 :*** If the nodes c_1 and c_2 are chosen such that they satisfy the equation

  $$\frac{1}{3} - \frac{1}{2}(c_1 + c_2) + c_1 c_2 = 0,$$

  then the corresponding method has order at least of 3, with Gaussian nodes or Radau nodes.

In addition to the energy preservation, the symmetry property of this method is also a crucial property. In general, symmetry of a method is defined in the following way:

Definition 3.3 *The numerical method $y_{n+1} = \phi_h(y_n)$ is said to be symmetric, if the system satisfies $\phi_h^{-1} = \phi_{-h}$.*

The symmetry condition of the energy preserving collocation method (3.10) given with the coefficients (3.11) is

$$a(1 - \xi, 1 - \eta) + a(\xi, \eta) = b(\eta),$$

which corresponds to

$$\sum_{i=1}^{s} \frac{1}{b_i} \left(l_i(\tau) l_i(\xi) - l_i(1 - \tau) l_i(1 - \xi)\right) = 0.$$

For the AVF method (3.3), symmetry can also be shown by the replacement of

$$\Delta t \to -\Delta t, \quad u^n \to u^{n+1}, \quad \text{and} \quad u^{n+1} \to u^n.$$

Despite the energy preserving and symmetry properties of the method, there is a problem that the method can not be both energy preserving and symplectic. As an alternative for the method not being symplectic, the concept of conjugate-symplecticity arisen, which means

that the method can be conjugate to a symplectic integrator up to an order. In [27], it is offered that if a change of coordinates $\psi_h(y) = y + O(h^{2s})$ is applied to the method, where $2s$ is the order of the energy-preserving collocation method, then $\psi_h^{-1}\,\phi_h\,\psi_h$ behave as a symplectic integrator in the long term. However, as checking conjugate symplecticity with this idea is hard to apply, a weaker definition may be given.

Definition 3.4 *The method $y_{n+1} = \phi_h(y_n)$ having order r is said to be **conjugate-symplectic** up to order q, where $q > r$, if under the change of coordinate $\psi_h(y) = y + O(h^r)$, where the Jacobian matrix*

$$\chi_h = \psi_h^{-1}\,\phi_h\,\psi_h$$

satisfies the equation

$$\chi_h(y)\,J\,\chi_h(y) = J + O(h^{q+1}).$$

Then the method acts as the symplectic integrator on the interval, which has length of h^{r-q}.

According to [27], the energy preserving method of order $2s$ is conjugate-symplectic up to order $2s + 2$, which shows the fact that the symplecticity property is achieved by the energy preserving methods up to an order.

3.3 AVF Method for Non-Canonical Hamiltonian Systems

This method is developed again using the same idea as the AVF method (3.3). It can be defined as [15]

$$\frac{u^{n+1} - u^n}{\Delta t} = J\left(\frac{u^n + u^{n+1}}{2}\right)\int_0^1 \nabla H((1-\tau)u^n + \tau u^{n+1})\,d\tau, \tag{3.12}$$

where the original problem is the Hamiltonian system (2.10).

This method is a general result for any type of the Jacobian, J. In particular, it is simplified to the energy preserving collocation integrator (3.3), if the matrix J is constant.

In addition to the energy preservation property of the previously introduced method (3.7), the developed version (3.12) preserves the Casimir functions; the implementation of this numerical integrator is similar to (3.7) with an exception in the Jacobian due to the u dependency:

$$y(t_0) = u_0 \tag{3.13}$$

$$\dot{y}(t_0 + c_i\Delta t) = J(y(t_0 + c_i\Delta t))\int_0^1 \frac{l_i(\tau)}{b_i}\nabla H(y(t_0 + \tau\Delta t))\,d\tau. \tag{3.14}$$

The next step is updated as $u_1 = y(t_0 + h)$, where $l_i(\tau)$ and b_i are same as (3.6).

This method can be reformulated identically as the integrator in [27] with a change of notation for Poisson systems. When we use the notation $K_\tau := y(t_0 + \tau\Delta t)$ and $K_i := y(t_0 + c_i\Delta t)$, Lagrange interpolation leads to

$$\dot{y}(t_0 + c_i\Delta t) = \sum_{i=1}^{s} l_i(\tau) J(K_i) \int_0^1 \frac{l_i(\tau)}{b_i} \nabla H(K_\tau)\, d\tau \tag{3.15}$$

and integrating (3.15) gives

$$K_\tau = u_0 + \Delta t \sum_{i=1}^{s} \int_0^1 \left(\frac{l_i(\tau)}{b_i} \int_0^\tau l_i(\alpha)\, d\alpha \right) J(K_i) \nabla H(K_\tau)\, d\tau. \tag{3.16}$$

The s degree polynomial $y(t)$ can be written in terms of u_0 and $K_1, \ldots, K_s$. Hence, the equation (3.16) is needed to compute the polynomial $y(t)$. That leads to a non-linear system of equations as in the previous case for the canonical Hamiltonian systems and can be solved by iterative methods. The method is equivalent to the implicit s-stage Runge-Kutta method (3.10) in its complexity. With the help of the AVF method, it can be shown that Runge-Kutta methods also preserves energy under special conditions. For more detailed information see [12].

The method introduced by (3.15) and (3.16) is again energy preserving because of the skew-symmetry property of $J(u)$. The energy is said to be preserved if

$$\frac{H(y(t_0 + \Delta t)) - H(y(t_0))}{\Delta t} = 0,$$

that is, if

$$\int_0^1 \nabla H(y(t_0 + \tau\Delta t))^T\, \dot{y}(t_0 + \tau\Delta t)\, d\tau = 0. \tag{3.17}$$

When the derivative of $y(t)$ is replaced by (3.15), the left hand side of (3.17) becomes

$$\sum_{i=1}^{s} b_i \left(\int_0^1 \frac{l_i(\tau)}{b_i} \nabla H(y(t_0 + \tau\Delta t)\, d\tau \right)^T J(K_i) \left(\int_0^1 \frac{l_i(\eta)}{b_i} \nabla H(y(t_0 + \eta\Delta t)\, d\eta \right),$$

which vanishes by the skew-symmetry of the matrix $J(K_i)$.

This method is claimed to preserve also the quadratic Casimir functions (2.1), which can be also defined as the function C(u) such that $\nabla C(u)^T J(u) = 0$, $\forall u$. The constant Casimir functions are clearly conserved for any Hamiltonian, since $\dfrac{dC(u)}{dt} = 0$.

Theorem 3.5 ([15]) *The Casimir function $C(u)$ of the form $C(u) = u^T M u$, where M is a constant matrix, is preserved up to order $2s$ with the energy preserving method based on the Gaussian quadrature formula.*

Proof. By the fundamental theorem of calculus

$$\frac{C(y(t_0+\Delta t))-C(y(t_0))}{\Delta t}=\int_0^1 \nabla C(y(t_0+\tau\Delta t))^T\,\dot{y}(t_0+\tau\Delta t)\,d\tau.$$

Applying the Gaussian quadrature with nodes b_i, c_i for $i = 1,\dots,s$, the difference $C(u_1) - C(u_0)$ is obtained as

$$\Delta t\sum_{i=1}^{s} b_i\nabla C(y(t_0+c_i\Delta t))^T J(y(t_0+c_i\Delta t))\int_0^1 \frac{l_i(\tau)}{b_i}\nabla H(y(t_0+\tau\Delta t)\,d\tau,$$

which vanishes due to skew-symmetry of J. ∎

The AVF methods (3.12) for non-canonical Hamiltonian systems (3.1) is a pseudo Poisson integrator [15].

3.4 Energy Preserving B-series Integrators

More recently, much attention has been given to a more general class of integrators, which include the Runge-Kutta methods as a subclass, which are the so-called B-series methods. The B-series methods are expressed in terms of rooted trees, that are a type of combinatorial graph and related with the vector field of the original differential equation. The conditions to conserve the quantities of the equation, such as symplecticity and energy preservation are examined using the rooted trees. The B-series methods can not be both Hamiltonian and energy preserving at the same time [6]. Therefore, some linear combinations of the rooted trees result in Hamiltonian B-series, while other linear combinations give energy preserving B-series. However, the energy preserving B-series can be conjugate to Hamiltonian B-series by the introduction of other B-series, which are called conjugate-Hamiltonian B-series or vice versa [57]. The conjugacy conditions are again expressed in terms of the rooted trees.

In general, B-series method enables numerical solution to be written in terms of rooted trees, which can be then expanded into B-series. The Taylor series methods and all Runge-Kutta methods are B-series.

The methods that we examined theoretically are structure preserving. However, insisting on structure preservation results in expensive computations or forces us to exclude other efficient numerical integrators with some other good long term properties. To make a connection of these methods, alternatively, with B-series methods the concept of *conjugacy* can be thought again, like we introduced for AVF methods.

Let the numerical integrator be represented as the map $\phi_{\Delta t}$ and let $\chi_{\Delta t}$ be another simpler integrator. Then if a map

$$\bar{\phi}_{\Delta t} = \chi_{\Delta t} \circ \phi_{\Delta t} \circ \chi_{\Delta t}^{-1}$$

is constructed as the conjugate scheme and applied N times to examine the long term behavior, the result

$$\bar{\phi}_{\Delta t}^{N} = \left(\chi_{\Delta t} \circ \phi_{\Delta t} \circ \chi_{\Delta t}^{-1}\right)^{N} = \chi_{\Delta t} \circ \phi_{\Delta t}^{N} \circ \chi_{\Delta t}^{-1}$$

shows that the two conjugate methods are independent of the number of steps taken. This shows that with a simpler integrator a conjugacy may be obtained and the structure preservation can be provided.

After the implementation of the AVF method, the existence of energy preserving B-series methods and the fact that the AVF method is a B-series method are shown in details in [13].

3.5 Modified Equations

The obtained solutions for the differential equations using numerical methods are always needed to be developed, in terms of the order or the properties of the methods. One way to obtain better results is to modify the differential equations with a perturbation in the equation. The idea of the modified equation is a result of the need of a backward error analysis. Usually the difference between the approximate and the exact solutions of the differential equation is examined to check the efficiency of the method, which corresponds to the forward error. However, if we can find a modified equation to the original one, then the local truncation error of the method can be found by taking the difference between the original and the modified equations. Therefore, for a rigorous treatment, the modified equation has to be truncated, so that the error can be made exponentially small and that leads to validity for long time intervals.

For a general differential equation $\dot{u} = f(u)$, the modified vector field is defined as $\tilde{f}(u)$, where the first term in the modified vector field is $f(u)$ and the next term is the leading term of the local truncation error of the method.

The modified differential equation $\dot{u} = \tilde{f}(u)$ is discussed in [28] and the Taylor expansion of

the exact solution of the modified equation $\tilde{f}(u)$ is given for a fixed t by

$$u(t+\Delta t) = u(t) + \Delta t\, \tilde{f}(u) + \frac{\Delta t}{2}\,(\tilde{f})'\,\tilde{f}(u) + \dots.$$

The modified equations are also applicable for the Hamiltonian system of differential equations, such that Hamiltonian operator or the Hamiltonian functional can be modified. However, for energy preservation of the method, only the operator should be modified without violating the self-adjointness property [13]. In [49], it is observed that the AVF method (3.3) defined for canonical type of Hamiltonian ode's is an energy-preserving B-series method, not a Runge-Kutta method. In its original form, the method has order 2. In order to obtain order 4, the method can be extended for (3.1) as follows:

$$\frac{u^{n+1}-u^n}{\Delta t} = \left(I - \frac{1}{12}(\Delta t)^2 f'\left(\frac{u^n+u^{n+1}}{2}\right)^2\right)\int_0^1 f\left((1-\tau)u^n + \tau u^{n+1}\right)\,d\tau.$$

This is also a skew-gradient method and in particular, the structure matrix J is modified here. That is, the method becomes

$$\frac{u^{n+1}-u^n}{\Delta t} = \tilde{J}\,\overline{\nabla} H_{AVF}(u^n, u^{n+1})$$

and this results in a modified structure matrix $\tilde{J}$ such that

$$\tilde{J} = \left(I - \frac{1}{12}(\Delta t)^2 f'\left(\frac{u^n+u^{n+1}}{2}\right)^2\right) J = J - \frac{1}{12}(\Delta t)^2 J\,\mathrm{Hess}(J).$$

We have also used the idea of modified equation by following the formulation in [24] for the KdV equation (2.14).

The general Hamiltonian system can be written as

$$u_t = \mathcal{J}\frac{\delta \mathcal{H}}{\delta u} \quad \text{or equivalently, in semi discrete form} u_t = \bar{J}(u)\nabla\bar{H}(u).$$

Let the modified equation be

$$y_t = \bar{J}(y)\nabla\bar{H}(y) + \Delta t\, A(y), \tag{3.18}$$

where $A(y)$ is the perturbation for the original equation.

In order to obtain the leading term of the truncation error, $A(y)$, the modified equation is expanded with Taylor series up to order 3, since the AVF method itself is of order 2, where

$$y(t+\Delta t) = y(t) + \Delta t\frac{\partial y(t)}{\partial t} + \frac{(\Delta t)^2}{2}\frac{\partial^2 y(t)}{\partial t^2} + O(3). \tag{3.19}$$

We know $\frac{\partial y(t)}{\partial t}$ from our assumption and taking its derivative gives

$$\frac{\partial^2 y(t)}{\partial t^2} = \frac{\partial}{\partial t}\Big(\bar{J}(y)\nabla\bar{H}(y) + \Delta t\, A(y)\Big) = \left(\frac{\partial}{\partial y}\Big(\bar{J}(y)\nabla\bar{H}(y) + \Delta t\, A(y)\Big)\right)\Big(\bar{J}(y)\nabla\bar{H}(y) + \Delta t\, A(y)\Big),$$

which results in

$$\frac{\partial^2 y(t)}{\partial t^2} = \left(\frac{\partial}{\partial y}\Big(\bar{J}(y)\nabla\bar{H}(y)\Big)\right)\Big(\bar{J}(y)\nabla\bar{H}(y)\Big)$$

by ignoring the higher order terms. If we substitute the derivatives into (3.19), we obtain

$$\begin{aligned} y(t+\Delta t) &= y(t) + \Delta t\Big(\bar{J}(y)\nabla\bar{H}(y) + \Delta t\, A(y)\Big) \\ &+ \frac{(\Delta t)^2}{2}\left(\frac{\partial}{\partial y}\Big(\bar{J}(y)\nabla\bar{H}(y)\Big)\right)\Big(\bar{J}(y)\nabla\bar{H}(y)\Big) + O(3). \end{aligned}$$

Since the order of the AVF method is 2, to satisfy it for the modified equation, $A(y)$ can be found as

$$A(y) = -\frac{1}{2}\left(\frac{\partial}{\partial y}\Big(\bar{J}(y)\nabla\bar{H}(y)\Big)\right)\Big(\bar{J}(y)\nabla\bar{H}(y)\Big)$$

and the semi-discrete modified equation (3.18) becomes

$$y_t = \bar{J}(y)\nabla\bar{H}(y) - \frac{\Delta t}{2}\left(\frac{\partial}{\partial y}\Big(\bar{J}(y)\nabla\bar{H}(y)\Big)\right)\Big(\bar{J}(y)\nabla\bar{H}(y)\Big).$$

When the modified formulation is applied to the semi-discrete first formulation of the KdV equation, where the first formulation [47] is given in terms of differential operators as

$$\mathcal{J}_1 = D, \quad \mathcal{H}_2 = \int\left(\frac{\alpha}{6}u^3 + \frac{\rho}{2}u^2 - \frac{\nu}{2}u_x^2\right)dx,$$

we can find the modified equation for the first pair as

$$y_t = \bar{J}_1(y)\nabla\bar{H}_2(y) - \frac{\Delta t}{2}\left(\bar{J}_1(y)\frac{\partial}{\partial y}\Big(\nabla\bar{H}_2(y)\Big)\right)\Big(\bar{J}_1(y)\nabla\bar{H}_2(y)\Big),$$

since the operator and the semi-discrete form are not dependent on y and this leads to the final modified equation

$$y_t = \tilde{\mathcal{J}}_1\mathcal{H}_2,$$

where

$$\tilde{\mathcal{J}}_1 = D - \frac{\Delta t}{2}D\Big(\nu D^2 + \alpha y + \rho\Big)D.$$

As offered in [49], the modified equation is obtained by only changing the operator. At that point, applying the AVF method to the modified equation will facilitate to do the backward error analysis of the method.

However, the modified equation can not be applied for the second Hamiltonian formulation $\mathcal{J}_2, \mathcal{H}_1$ of the KdV system, because the resulting equation can not be written as

$$y_t = \tilde{\mathcal{J}}_2 \mathcal{H}_1$$

keeping the Hamiltonian as original and modifying the Hamiltonian operator.

CHAPTER 4

APPLICATION OF AVERAGE VECTOR FIELD INTEGRATOR TO KdV TYPE EQUATIONS

The theory behind the Hamiltonian systems has been investigated in Chapter 2, where the concept of bi-Hamiltonian equations is introduced,too. In this chapter, we apply the energy preserving AVF method to the bi-Hamiltonian equations, such as Korteweg de Vries (KdV), modified Korteweg de Vries (mKdV), Ito system and two different coupled KdV-KdV system. First, the two Hamiltonian PDEs are discretized in space by preserving the skew-symmetric structure of the underlying PDEs and the resulting ODEs and solved using the AVF method. Because the energy preserving AVF method is implicit, the resulting implicit nonlinear equations are solved by Newton iteration within machine accuracy.

4.1 Formulation of the Bi-Hamiltonian Equations

4.1.1 Korteweg de Vries Equation

The KdV equation has a deep history, as a strong example for solitary waves and solitons. The origin of the KdV equation is in [34], where the equation is first found as the shallow water waves, which became a model for atmospheric fluid dynamics, with the constants $\alpha = -6$, $\rho = 0$ and $\nu = -1$. The shallow water waves were modeled as KdV equations with a sixty years of gap after the Scott Russell's observations of wave translation [50] in the Edinburgh-Glasgow canal. Another detailed derivation of the KdV equation can be obtained using the starting point of the governing equations of motion of an ideal fluid, which is introduced in [59].

The KdV type equations are generally named as solitons. The concept of the solitons for the KdV equations was first introduced by Zabusky and Kruskal [62] in 1965. The name of solitons is used for the waves with particle property. Here, the particle property means that interaction of any two or more waves does not lead to any deformation in the shape or speed of the waves, but the phases are shifted. In addition to the soliton property of the KdV equations, some of the conserved quantities of the KdV equation are obtained in [43].

With the invention of the equation and its properties, various methods are tried to solve the KdV equation exactly [10], whereas the first implemented one was inverse scattering method, which is introduced in [21].

KdV equation is governing weakly, nonlinear long waves whose phase speed reaches a maximum for waves of infinite length. It arises in the study of solitary waves, basically in the physical models of atmosphere and ocean motion, mid-latitude and equatorial planetary waves, ion-acoustic waves in plasma, lattice waves, waves in elastic rods, pressure waves in a liquid-gas bubble mixture. (See, for example, [18, 38, 45, 58].)

The general KdV equation, which was also presented in (2.14)

$$u_t = \alpha u u_x + \rho u_x + \nu u_{xxx}.$$

The bi-Hamiltonian form of the KdV equation (2.14) is given in [47] as

$$\mathcal{J}_1 = D, \quad \mathcal{J}_2 = \frac{\alpha}{3} u D + \frac{\alpha}{3} D u + \rho D + \nu D^3, \tag{4.1}$$

$$\mathcal{H}_1 = \int \frac{1}{2} u^2 dx, \quad \mathcal{H}_2 = \int \left(\frac{\alpha}{6} u^3 + \frac{\rho}{2} u^2 - \frac{\nu}{2} u_x^2 \right) dx. \tag{4.2}$$

In order to apply the AVF method, the skew-adjoint operators $\mathcal{J}_1$ and $\mathcal{J}_2$ and the Hamiltonians $\mathcal{H}_1$ and $\mathcal{H}_2$ have to be discretized in space. The most important aspect of the semi-discretization in space is the preservation of the skew-adjoint (skew-symmetric) structure of the operators $\mathcal{J}_1$ and $\mathcal{J}_2$ [14, 39]. The skew adjoint operator $\mathcal{J}_1 = D$ of the first Hamiltonian pair is discretized as $Du = \frac{u_{j+1} - u_j}{2\Delta x}$ by using central difference. Hence, $\mathcal{J}_1$ becomes

$$\bar{J}_1 = \frac{1}{2\Delta x} A, \quad \text{where} \quad A = \begin{pmatrix} 0 & 1 & & & -1 \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ 1 & & & -1 & 0 \end{pmatrix} \tag{4.3}$$

and A is an $N \times N$ circulant tridiagonal matrix.

The discretization of the Hamiltonian functional $\mathcal{H}_2$ is not needed to be skew-symmetric unlike the Hamiltonian operator $\mathcal{J}_1$. Many different discretizations, such as backward or forward are accepted for a Hamiltonian functional, and some of these are offered in [17]. In this work, for the Hamiltonian functional of the first pair, $\mathcal{H}_2$, and for all of the remaining functionals of the KdV-type equations in this Chapter, we will use the forward difference;

$$\bar{H}_2 = \sum_{j=1}^{N} \left(\frac{\alpha}{6} u_j^3 + \frac{\rho}{2} u_j^2 - \frac{\nu}{2\Delta x^2} (u_{j+1} - u_j)^2 \right) \Delta x, \tag{4.4}$$

where u_j is an element of the N dimensional vector u such that $u = (u_1, \ldots, u_N)^T$. The integral $\bar{H}_1$ is discretized by the well-known rectangle rule.

The gradient of the discrete Hamiltonian (4.4) is then

$$\nabla \bar{H}_2(u_j) = \frac{\alpha}{2} u_j^2 + \rho u_j + \frac{\nu}{\Delta x^2} (u_{j+1} - 2u_j + u_{j-1}), \quad \text{for} \quad j = 1, \ldots, N, \tag{4.5}$$

where $\nabla \bar{H}_2(u)$ is an N dimensional vector.

After applying the AVF method (3.12), we obtain the system of ODEs

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{\alpha}{12\Delta x} A \left[(u^n)^2 + diag(u^n) u^{n+1} + (u^{n+1})^2 \right] + \frac{\rho}{4\Delta x} A \left(u^n + u^{n+1} \right) + \frac{\nu}{4\Delta x^3} A \left(\tilde{u}^n + \tilde{u}^{n+1} \right), \tag{4.6}$$

with

$$u^n = (u_1^n, \ldots, u_j^n, \ldots, u_N^n)^T, \tag{4.7}$$

$$\tilde{u}^n = (u_2^n - 2u_1^n + u_N^n, \ldots, u_{j+1}^n - 2u_j^n + u_{j-1}^n, \ldots, u_1^n - 2u_N^n + u_{N-1}^n)^T \tag{4.8}$$

where *diag* represents diagonal matrix of dimension $N \times N$ with elements of the vector u^n on the main diagonal.

The implicit system of equations (4.6) can be written as

$$F(u^{n+1}) = 0. \tag{4.9}$$

The Newton's method then can be applied to (4.9) as

$$J_F(u_\kappa^{n+1}) \left(u_{\kappa+1}^{n+1} - u_\kappa^{n+1} \right) = -F(u_\kappa^{n+1}), \tag{4.10}$$

where $J_F(u_\kappa^{n+1})$ is the Jacobian of the function $F(u_\kappa^{n+1})$. Solving (4.10) for $u_{\kappa+1}^{n+1}$ at each step with a tolerance, will give the approximation to the equation. In the calculation, κ represents

the iteration level for Newton's method. In the computation, because the linear system of equations to be solved during the Newton iteration are sparse and have block tridiagonal form, sparse matrix solvers of MATLAB is used.

Introducing the constants $r = \Delta t/4\Delta x^3$ and $s = \Delta t/12\Delta x$, the corresponding Jacobian can be obtained as

$$\bar{J_F}(u^{n+1}) = I - s\alpha(A\,R(u^n)) - s\alpha(A\,Q(u^{n+1})) - 3s\rho A - r\nu(A\,P), \tag{4.11}$$

which is found by taking the derivative of the equation (4.6) with respect to u^{n+1}.

The square matrices R, Q, P are

$$R(u^n) = diag(u^n), \quad Q(u^{n+1}) = diag(2\,u^{n+1}),$$

where *diag* is used to represent the diagonal matrix with the given vector elements on the main diagonal and the constant matrix P can be written as

$$P = \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 1 & & & 1 & -2 \end{pmatrix}. \tag{4.12}$$

The implicit equation (4.6) has to be solved within the machine accuracy. We have used therefore as stopping criteria for Newton's method tolerance between $10^{-13} - 10^{-15}$.

The formulation of the second Hamiltonian pair $\mathcal{J}_2$ and $\mathcal{H}_1$ for the KdV equation can be done similar to the first formulation. The skew-adjoint operator for the second Hamiltonian pair is more complicated then in the first formulation. But this is compensated by a simpler Hamiltonian functional in the formulation.

The semi-discretized $\mathcal{J}_2$ is given as

$$\bar{J_2} = \frac{\alpha}{6\Delta x}C(u) + \frac{\rho}{2\Delta x}A + \frac{\nu}{2\Delta x^3}B, \tag{4.13}$$

where the matrix A is same as (4.3) in the first formulation. The matrix $C(u)$ can be defined

as

$$C(u) = \begin{pmatrix} 0 & u_1+u_2 & & -(u_1+u_N) \\ -(u_2+u_1) & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}+u_N \\ u_N+u_1 & & -(u_N+u_{N-1}) & 0 \end{pmatrix}, \tag{4.14}$$

which is the discretization of the term $\frac{\alpha}{3}uD+\frac{\alpha}{3}Du$ of $\mathcal{J}_2$. The terms uD and Du are discretized together in one matrix in order not to violate the self-adjointness of the operator as offered in [39]. The matrix B

$$B = \begin{pmatrix} 0 & -2 & 1 & & -1 & 2 \\ 2 & \ddots & \ddots & \ddots & & -1 \\ -1 & \ddots & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & 1 \\ 1 & & \ddots & \ddots & \ddots & -2 \\ -2 & 1 & & -1 & 2 & 0 \end{pmatrix}, \tag{4.15}$$

corresponds to the discrete D^3 in the operator $\mathcal{J}_2$, so the constant entries of the matrix B are the coefficients of the vector elements u_j in the central discretization of u_{xxx} as in [3]

$$u_{xxx} = \frac{u_{j+2} - 2u_{j+1} + 2u_{j-1} - u_{j-2}}{\Delta x^3}.$$

The Hamiltonian functional $\mathcal{H}_1$ of the second Hamiltonian pair can be discretized simply as

$$\bar{H}_1 = \sum_{j=1}^{N} \frac{1}{2} u_j^2 \Delta x, \tag{4.16}$$

then the gradient of the discrete Hamiltonian functional is clearly $\nabla \bar{H}_1 = u$, which is the N dimensional vector.

Applying the AVF method yields

$$\frac{u^{n+1}-u^n}{\Delta t} = \left(\frac{\alpha}{12\Delta x}C(u^n) + \frac{\alpha}{12\Delta x}C(u^{n+1}) + \frac{\rho}{2\Delta x}A + \frac{\nu}{2\Delta x^3}B\right) \cdot \left(\frac{1}{2}\left(u^{n+1}+u^n\right)\right), \tag{4.17}$$

where $C(u^n)$ and $C(u^{n+1})$ have the same entries as the matrix (4.14), but they are evaluated at the time level of n and $n+1$, respectively. Introducing the constant $r = \Delta t/4\Delta x^3$, $s = \Delta t/12\Delta x$ and taking the derivative of (4.17) with respect to u^{n+1}, the Jacobian, which is used to solve the system with the Newton's method, is obtained as

$$\bar{J}_F(u^{n+1}) = I - s\alpha G(u^n) - s\alpha D(u^{n+1}) - s\alpha E(u^n) - 6s\rho A - r\nu B. \tag{4.18}$$

The square $N \times N$ matrices in (4.18) are

$$D(u^{n+1}) = \begin{pmatrix} u_2^{n+1} - u_N^{n+1} & 2u_2^{n+1} & & -2u_N^{n+1} \\ -2u_1^{n+1} & \ddots & \ddots & \\ & \ddots & \ddots & 2u_N^{n+1} \\ 2u_1^{n+1} & & -2u_{N-1}^{n+1} & u_1^{n+1} - u_{N-1}^{n+1} \end{pmatrix}$$

and

$$E(u^n) = \begin{pmatrix} u_2^n - u_N^n & u_2^n & & -u_N^n \\ -u_1^n & \ddots & \ddots & \\ & \ddots & \ddots & u_N^n \\ u_1^n & & -u_{N-1}^n & u_1^n - u_{N-1}^n \end{pmatrix}. \tag{4.19}$$

The solutions of the KdV equation (2.14) with respect to both of the Hamiltonian formulations (4.1) and (4.2) with the AVF method (3.12) are examined in the next chapter.

4.1.2 Modified Korteweg de Vries Equation

We consider the general modified KdV (mKdV) equation

$$u_t = -\alpha u^2 u_x - \beta u_{xxx}. \tag{4.20}$$

The mKdV equations belong to the category of completely integrable systems as the KdV equations [63] and they all admit soliton solutions. The mKdV equation can be derived from the KdV equations using Miura transformations [25]:

$$u = -v_x - v^2.$$

Then the mKdV equation is obtained for $\alpha = 6$ and $\beta = 1$ as

$$v_t + 6v^2 v_x + v_{xxx} = 0.$$

The bi-Hamiltonian structure of the general mKdV equation is given in [47], where the Hamiltonian pairs are given for the case $\alpha = -3/2$ and $\nu = 1$. When we rewrite it for general equation(4.20), the bi-Hamiltonian formulation becomes

$$\mathcal{J}_1 = D, \quad \mathcal{J}_2 = -\frac{2\alpha}{3} DuD^{-1}uD - \beta D^3 \tag{4.21}$$

$$\mathcal{H}_1 = \int \frac{1}{2}u^2 dx, \quad \mathcal{H}_2 = \int \left(-\frac{\alpha}{12}u^4 - \frac{\beta}{2}u_x^2\right) dx. \tag{4.22}$$

However the term D^{-1} in the second Hamiltonian operator $\mathcal{J}_2$ represents integral and prevents us from writing the finite difference for $\mathcal{J}_2$. Therefore, to get rid of the term D^{-1}, the integral operator is applied to u from right and we obtain the second Hamiltonian operator as

$$\mathcal{J}_2 = -\frac{2\alpha}{3} D \frac{u^3}{2} D - \beta D^3.$$

Since our aim is to obtain the term $-\alpha u^2 u_x$ in the mKdV equation with

$$u_t = \mathcal{J}_2 \frac{\delta \mathcal{H}_1}{\delta u},$$

the final version of $\mathcal{J}_2$ is

$$\mathcal{J}_2 = -\frac{\alpha}{2} u D u - \beta D^3,$$

where the new Hamiltonian formulation can be rewritten as

$$\mathcal{J}_1 = D, \quad \mathcal{J}_2 = -\frac{\alpha}{2} u D u - \beta D^3 \tag{4.23}$$

$$\mathcal{H}_1 = \int \frac{1}{2} u^2 dx, \quad \mathcal{H}_2 = \int \left(-\frac{\alpha}{12} u^4 - \frac{\beta}{2} u_x^2 \right) dx. \tag{4.24}$$

The new formulation of $\mathcal{J}_2$ is rewritten such that the skew symmetry is preserved in the discrete form.

Now we can apply the AVF method (3.12) to the general mKdV equation (4.20) using the Hamiltonian pairs $\mathcal{J}_1, \mathcal{H}_2$ and $\mathcal{J}_2, \mathcal{H}_1$.

The skew-adjoint operator $\mathcal{J}_1$ is easy to discretize and it is that of the same as $\bar{J}_1$ in (4.3). Then the discrete case of the Hamiltonian is

$$\bar{H}_2 = \sum_{j=1}^{N} \left(-\frac{\alpha}{12} u_j^4 + \frac{\beta}{2\Delta x^2} (u_{j+1} - u_j)^2 \right) \Delta x, \tag{4.25}$$

with the gradient

$$\nabla \bar{H}_2(u_j) = -\frac{\alpha}{3} u_j^3 - \frac{\beta}{\Delta x^2} (u_{j+1} - 2u_j + u_{j-1}). \tag{4.26}$$

Applying the AVF method gives the equation

$$\begin{aligned} \frac{u^{n+1} - u^n}{\Delta t} = & - \frac{\alpha}{24\Delta x} A \left[(u^n)^3 + diag((u^n)^2) u^{n+1} + diag(u^n)(u^{n+1})^2 + (u^{n+1})^3 \right] \\ & - \frac{\beta}{4\Delta x^3} A \left[\tilde{u}^n + \tilde{u}^{n+1} \right], \end{aligned} \tag{4.27}$$

where *diag* represents $N \times N$ dimensional diagonal matrix, $\tilde{u}^n$ is same as (4.8) and the vector $\tilde{u}^{n+1}$ is the upper time level of $\tilde{u}^n$. The function $F(u^{n+1})$ can be deduced and the resulting Jacobian for the Newton's method is

$$J_F(u^{n+1}) = I + s\alpha(A\, Q(u^n)) + s\alpha(A\, Q(u^n, u^{n+1})) + s\alpha(A\, T(u^{n+1})) + r\beta(A\, P), \tag{4.28}$$

where $s = \Delta t/24\Delta x$ and $r = \Delta t/4\Delta x^3$. The matrices A, P, Q, R and T are all N dimensional square matrices, where A and P are equal to (4.3) and (4.12), respectively, and the others can be written as

$$Q(u^n) = diag((u^n)^2), \quad R(u^n, u^{n+1}) = diag(2u^n u^{n+1}), \quad \text{and} \quad T(u^{n+1}) = diag(3(u^{n+1})^2).$$

The second Hamiltonian formulation can be obtained in a similar manner since

$$\bar{H}_1 = \sum_{j=1}^{N} \frac{1}{2} u_j^2 \Delta x \quad \text{and} \quad \nabla \bar{H}_1(u_j) = u_j \quad \text{for} \quad j = 1, \ldots, N.$$

Then the operator $\bar{J}_2$ has the discretized form of

$$\bar{J}_2 = -\frac{\alpha}{4\Delta x} C(u) - \frac{\beta}{2\Delta x^3} B,$$

where B is same as the matrix (4.15) and

$$C(u) = \begin{pmatrix} 0 & u_1u_2 & & -u_1u_N \\ -u_2u_1 & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}u_N \\ u_Nu_1 & & -u_Nu_{N-1} & 0 \end{pmatrix}. \tag{4.29}$$

Here, the matrix $C(u)/2\Delta x$ is the discrete version of the term uDu in the Hamiltonian operator. It is obtained from the discretization of the term uDu in $\mathcal{J}_2$ as $\frac{1}{2\Delta x} u^T A u$, where A is the matrix (4.3) and u is N dimensional vector.

To apply the AVF method, since $\bar{J}_2$ is dependent on u, it has to be evaluated at $\frac{u^n + u^{n+1}}{2}$, which gives

$$\bar{J}_2\left(\frac{u^n + u^{n+1}}{2}\right) = -\frac{\alpha}{16\Delta x}\left(G(u^n) + G(u^{n+1}) + E(u^n, u^{n+1}) + F(u^n, u^{n+1})\right) - \frac{\beta}{2\Delta x^3} B,$$

where the matrices $G(u^n)$ and $G(u^{n+1})$ are equal to the matrix (4.29) with the entries calculated at the time level n and $n+1$, respectively. The matrices E, F are

$$E(u^n, u^{n+1}) = \begin{pmatrix} 0 & u_1^n u_2^{n+1} & & -u_1^{n+1}u_N^n \\ -u_2^{n+1}u_1^n & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}^n u_N^{n+1} \\ u_N^n u_1^{n+1} & & -u_N^{n+1}u_{N-1}^n & 0 \end{pmatrix}$$

and

$$F(u^n, u^{n+1}) = \begin{pmatrix} 0 & u_1^{n+1}u_2^n & & -u_1^n u_N^{n+1} \\ -u_2^n u_1^{n+1} & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}^{n+1}u_N^n \\ u_N^{n+1}u_1^n & & -u_N^n u_{N-1}^{n+1} & 0 \end{pmatrix}.$$

The full discretized system becomes then

$$\begin{aligned} u^{n+1} - u^n = & - s\alpha\left(K(u^n) + K(u^{n+1})\right) - r\beta\left(M(u^n) + M(u^{n+1})\right) \\ & - 2s\alpha\left(P(u^n, u^{n+1}) + R(u^n, u^{n+1})\right) - s\alpha\left(Q(u^n, u^{n+1}) + T(u^n, u^{n+1})\right), \end{aligned} \tag{4.30}$$

with the constants $s = \Delta t/32\Delta x$ and $r = \Delta t/4\Delta x^3$, where the jth row of the N dimensional vectors are

$$\begin{aligned} K(u_j^n) &= u_j^n\left((u_{j+1}^n)^2 - (u_{j-1}^n)^2\right), \quad M(u_j^n) = u_{j+2}^n - 2u_{j+1}^n + 2u_{j-1}^n - u_{j-2}^n, \\ P(u_j^n, u_j^{n+1}) &= u_j^n\left(u_{j+1}^{n+1}u_{j+1}^n - u_{j-1}^{n+1}u_{j-1}^n\right), \quad R(u_j^n, u_j^{n+1}) = u_j^{n+1}\left(u_{j+1}^{n+1}u_{j+1}^n - u_{j-1}^{n+1}u_{j-1}^n\right), \\ Q(u_j^n, u_j^{n+1}) &= u_j^n\left((u_{j+1}^{n+1})^2 - (u_{j-1}^{n+1})^2\right), \quad T(u_j^n, u_j^{n+1}) = u_j^{n+1}\left((u_{j+1}^n)^2 - (u_{j-1}^n)^2\right). \end{aligned}$$

Using the equation (4.30), the Jacobian to solve the second formulation with the Newton's method can be acquired by taking the derivatives of the vectors K, M, P, R, Q and T with respect to u^{n+1} as

$$J_F(u^{n+1}) = I + s\alpha\left[C(u^{n+1}) + 2A(u^n) + 2D(u^n, u^{n+1}) + S(u^n, u^{n+1})\right] + r\beta B, \tag{4.31}$$

where B is equal to (4.15),

$$C(u^{n+1}) = \begin{pmatrix} (u_2^{n+1})^2 - (u_N^{n+1})^2 & 2u_1^{n+1}u_2^{n+1} & & -2u_1^{n+1}u_N^{n+1} \\ -2u_2^{n+1}u_1^{n+1} & \ddots & \ddots & \\ & \ddots & \ddots & 2u_{N-1}^{n+1}u_N^{n+1} \\ 2u_N^{n+1}u_1^{n+1} & & -2u_N^{n+1}u_{N-1}^{n+1} & (u_1^{n+1})^2 - (u_{N-1}^{n+1})^2 \end{pmatrix},$$

$$A(u^n) = \begin{pmatrix} 0 & u_1^n u_2^n & & -u_1^n u_N^n \\ -u_2^n u_1^n & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}^n u_N^n \\ u_N^n u_1^n & & -u_N^n u_{N-1}^n & 0 \end{pmatrix},$$

$$D(u^n, u^{n+1}) = \begin{pmatrix} u_2^{n+1}u_2^n - u_N^{n+1}u_N^n & u_1^{n+1}u_2^n & & -u_1^{n+1}u_N^n \\ -u_2^{n+1}u_1^n & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}^{n+1}u_N^n \\ u_N^{n+1}u_1^n & & -u_N^{n+1}u_{N-1}^n & u_1^{n+1}u_1^n - u_{N-1}^{n+1}u_{N-1}^n \end{pmatrix},$$

and

$$S(u^n, u^{n+1}) = \begin{pmatrix} (u_2^n)^2 - (u_N^n)^2 & 2u_1^n u_2^{n+1} & & -2u_1^n u_N^{n+1} \\ -2u_2^n u_1^{n+1} & \ddots & \ddots & \\ & \ddots & \ddots & 2u_{N-1}^n u_N^{n+1} \\ 2u_N^n u_1^{n+1} & & -2u_N^n u_{N-1}^{n+1} & (u_1^n)^2 - (u_{N-1}^n)^2 \end{pmatrix},$$

where the matrix $S(u^n, u^{n+1})$ is the sum of the derivatives of the vectors $Q(u^n, u^{n+1})$ and $T(u^n, u^{n+1})$ in (4.30).

The second formulation of the mKdV equation is more complex than the first one due to the complexity of the discrete form of the second Hamiltonian operator $\mathcal{J}_2$.

4.1.3 Ito's System

The Hamiltonian operator of the bi-Hamiltonian formulations of the coupled equations such as Ito's system become matrices when discretized contrary to the previously examined KdV type equations, since the solutions of the PDEs turn to coupled system of equations with two variables.

The original form of the equation proposed by Ito [32] is

$$u_{tt} = u_{xxxt} + (uu_t)_x + \left(u_x \int^x u_t dy\right)_x, \tag{4.32}$$

which can be written as a coupled system [36]. However, a more general way of writing (4.32) as a coupled system of equations is introduced in [61] as

$$u_t + \alpha u u_x + \beta v v_x + \gamma u_{xxx} = 0, \tag{4.33}$$

$$v_t + \beta (uv)_x = 0, \tag{4.34}$$

with the choice of $\alpha = -6, \beta = -2$ and $\gamma = -1$. Therefore, the bi-Hamiltonian formulation offered in [47] is revised as

$$\mathcal{J}_1 = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}, \quad \mathcal{J}_2 = \begin{pmatrix} uD + Du + \frac{1}{2}D^3 & vD \\ Dv & 0 \end{pmatrix},$$
$$\mathcal{H}_1 = \int \left(u^2 + v^2\right) dx, \quad \mathcal{H}_2 = \int \left(u^3 + uv^2 - u_x^2\right) dx,$$

where the one dimensional operators change to 2×2 matrix operators. To express the first formulation of the Ito's system using AVF method, let us start with the semi-discretization of the first Hamiltonian pair

$$\bar{J}_1 = \frac{1}{2\Delta x} \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}, \quad \bar{H}_2 = \sum_{j=1}^{N} \left(u_j^3 + u_j v_j^2 - \frac{1}{\Delta x^2}(u_{j+1} - u_j)^2\right) \Delta x, \tag{4.35}$$

where the matrix A is known from (4.3).

Then the gradient of $\bar{H}_2$, which is a vector of $2N$ dimensional such that

$$\nabla\bar{H}_2(u,v) = \begin{pmatrix} \frac{\partial\bar{H}_2}{\partial u} \\ \\ \frac{\partial\bar{H}_2}{\partial v} \end{pmatrix} = \begin{pmatrix} 3u_1^2 + v_1^2 + \frac{2}{\Delta x^2}(u_2 - 2u_1 + u_N) \\ \vdots \\ 3u_j^2 + v_j^2 + \frac{2}{\Delta x^2}\left(u_{j+1} - 2u_j + u_{j-1}\right) \\ \vdots \\ 3u_N^2 + v_N^2 + \frac{2}{\Delta x^2}(u_1 - 2u_N + u_{N-1}) \\ 2u_1v_1 \\ \vdots \\ 2u_jv_j \\ \vdots \\ 2u_Nv_N \end{pmatrix},$$

where $j = 1, \ldots, N$. Applying the AVF method results in the following equations, which are in the block matrix form

$$\begin{aligned} \frac{u^{n+1} - u^n}{\Delta t} &= \frac{1}{2\Delta x}A\left(\hat{u}^n + \frac{1}{3}\hat{v}^n\right) + \frac{1}{2\Delta x^3}A\left(\tilde{u}^n + \tilde{u}^{n+1}\right), \\ \frac{v^{n+1} - v^n}{\Delta t} &= \frac{1}{2\Delta x}A\left(\widetilde{uv}\right), \end{aligned}$$

where

$$\begin{aligned} v^n &= (v_1^n, \ldots, v_j^n, \ldots, v_N^n)^T, \\ \hat{u}^n &= ((u_1^n)^2 + u_1^n u_1^{n+1} + (u_1^{n+1})^2, \ldots, (u_j^n)^2 + u_j^n u_j^{n+1} + (u_j^{n+1})^2, \ldots, (u_N^n)^2 + u_N^n u_N^{n+1} + (u_N^{n+1})^2)^T, \\ \hat{v}^n &= ((v_1^n)^2 + v_1^n v_1^{n+1} + (v_1^{n+1})^2, \ldots, (v_j^n)^2 + v_j^n v_j^{n+1} + (v_j^{n+1})^2, \ldots, (v_N^n)^2 + v_N^n v_N^{n+1} + (v_N^{n+1})^2)^T, \\ \widetilde{uv} &= (\ldots, \frac{2}{3}u_j^n v_j^n + \frac{1}{3}\left(u_j^n v_j^{n+1} + u_j^{n+1} v_j^n\right) + \frac{2}{3}u_j^{n+1} v_j^{n+1}, \ldots)^T, \end{aligned}$$

the vectors $\tilde{u}^n$ is same as (4.8) and $\tilde{u}^{n+1}$ is the $n+1$th level of $\tilde{u}^n$.

When we take the derivative,the Jacobian is obtained as a block square matrix of dimension $2N$.

$$\bar{J}_F(u^{n+1}, v^{n+1}) = \left(\begin{array}{c|c} \bar{J}_{F1} & \bar{J}_{F2} \\ \hline \bar{J}_{F3} & \bar{J}_{F4} \end{array}\right), \tag{4.36}$$

where the matrix elements are $N \times N$ matrices such that

$$\begin{aligned} \bar{J}_{F1} &= I - 3rAdiag(2u^{n+1}) - 3rAdiag(u^n) - sAP, \\ \bar{J}_{F2} = \bar{J}_{F3} &= -rAdiag(2v^{n+1}) - rAdiag(v^n), \\ \bar{J}_{F4} &= I - rAdiag(2u^{n+1}) - 3rAdiag(u^n), \end{aligned}$$

where the constants are $s = \Delta t/2\Delta x^3$ and $r = \Delta t/6\Delta x$ and the matrices A and P are (4.3) and (4.12), respectively, as introduced before.

The second formulation is similar with a simple Hamiltonian but with a more complex operator. The semi-discrete operator is

$$\bar{J}_2 = \left(\begin{array}{c|c} \frac{1}{2\Delta x} C(u^n) + \frac{1}{2\Delta x^3} B & \frac{1}{2\Delta x} E(v^n) \\ \hline \frac{1}{2\Delta x} D(v^n) & 0 \end{array} \right).$$

The matrices $E(v^n)$, $D(v^n)$ are

$$E(v^n) = \begin{pmatrix} 0 & v_1^n & & -v_1^n \\ -v_2^n & \ddots & \ddots & \\ & \ddots & \ddots & v_{N-1}^n \\ v_N^n & & -v_N^n & 0 \end{pmatrix}, \quad D(v^n) = \begin{pmatrix} 0 & v_2^n & & -v_N^n \\ -v_1^n & \ddots & \ddots & \\ & \ddots & \ddots & v_N^n \\ v_1^n & & -v_{N-1}^n & 0 \end{pmatrix}, \tag{4.37}$$

B is equal to (4.15) and $C(u^n)$ has the same entries as (4.14), but evaluated at the nth time level. The matrices $E(v^n)$ and $D(v^n)$ satisfy the property $E(v^n)^* = -E(v^n)^T = D(v^n)$, which preserves the skew-symmetry of discrete $\bar{J}_2$.

The Hamiltonian is discretized as

$$\bar{H}_1 = \sum_{j=1}^{N} \left(u_j^2 + v_j^2 \right) \Delta x.$$

After applying the AVF method, we obtain

$$\begin{aligned} u^{n+1} - u^n &= s\left(M(u^n) + M(u^{n+1})\right) + r\left(K(u^n) + K(u^{n+1}) + N(v^n) + N(v^{n+1})\right) \\ &+ r\left(E(u^n, u^{n+1}) + F(u^n, u^{n+1}) + P(v^n, v^{n+1}) + S(v^n, v^{n+1})\right), \qquad (4.38) \\ v^{n+1} - v^n &= r\left(Q(u^n, v^n) + Q(u^{n+1}, v^{n+1}) + R(u^{n+1}, v^n) + T(u^n, v^{n+1})\right), \qquad (4.39) \end{aligned}$$

where $s = \Delta t/4\Delta x^3$, $r = \Delta t/4\Delta x$ and the jth row of the vectors are as the following

$$M(u_j^n) = u_{j+2}^n - 2u_{j+1}^n + 2u_{j-1}^n - u_{j-2}^n, \quad K(u_j^n) = u_{j+1}^n \left(u_{j+1}^n + u_j^n\right) - u_{j-1}^n \left(u_{j-1}^n + u_j^n\right),$$

$$E(u_j^n, u_j^{n+1}) = u_{j+1}^{n+1} \left(u_{j+1}^n + u_j^n\right) - u_{j-1}^{n+1} \left(u_{j-1}^n + u_j^n\right),$$

$$F(u_j^n, u_j^{n+1}) = u_{j+1}^n \left(u_{j+1}^{n+1} + u_j^{n+1}\right) - u_{j-1}^n \left(u_{j-1}^{n+1} + u_j^{n+1}\right),$$

$$P(v_j^n, v_j^{n+1}) = v_j^n \left(v_{j+1}^{n+1} - v_{j-1}^{n+1}\right), \quad S(v_j^n, v_j^{n+1}) = v_j^{n+1} \left(v_{j+1}^n - v_{j-1}^n\right),$$

$$Q(u_j^n, v_j^n) = u_{j+1}^n v_{j+1}^n - u_{j-1}^n v_{j-1}^n, \quad R(u_j^{n+1}, v_j^n) = u_{j+1}^{n+1} v_{j+1}^n - u_{j-1}^{n+1} v_{j-1}^n,$$

$$T(u_j^n, v_j^{n+1}) = u_{j+1}^n v_{j+1}^{n+1} - u_{j-1}^n v_{j-1}^{n+1},$$

for $j = 1, \ldots, N$.

The Jacobian in the form of block matrix is

$$J_F(u^{n+1}, v^{n+1}) = \begin{pmatrix} I - sB - rD(u^{n+1}) - rA(u^n) - rC(u^n) & -r\left(X(v^n) + X(v^{n+1})\right) \\ -r\left(Y(v^n) + Y(v^{n+1})\right) & I - r\left(Z(u^n) + Z(u^{n+1})\right) \end{pmatrix},$$

with B is same as (4.15) and

$$D(u^{n+1}) = \begin{pmatrix} u_2^{n+1} - u_N^{n+1} & 2u_2^{n+1} & & -2u_N^{n+1} \\ -2u_1^{n+1} & \ddots & \ddots & \\ & \ddots & \ddots & 2u_N^{n+1} \\ 2u_1^{n+1} & & -2u_{N-1}^{n+1} & u_1^{n+1} - u_{N-1}^{n+1} \end{pmatrix},$$

$$A(u^n) = \begin{pmatrix} 0 & u_1^n + u_2^n & & -(u_1^n + u_N^n) \\ -(u_2^n + u_1^n) & \ddots & \ddots & \\ & \ddots & \ddots & u_{N-1}^n + u_N^n \\ u_N^n + u_1^n & & -(u_N^n + u_{N-1}^n) & 0 \end{pmatrix},$$

$$X(v^n) = \begin{pmatrix} v_2^n - v_N^n & v_2^n & & -v_N^n \\ -v_1^n & \ddots & \ddots & \\ & \ddots & \ddots & v_N^n \\ v_1^n & & -v_{N-1}^n & v_1^n - v_{N-1}^n \end{pmatrix}.$$

The matrix $C(u^n)$ is equal to (4.19) and $Y(v^n)$ has same entries as $D(v^n)$ in (4.37). The last two matrices $Z(u^n)$ and $Z(u^{n+1})$ also have the same matrix elements as $D(v^n)$ in (4.37), but with the time level n and $n + 1$ for the solution u^n.

4.2 Coupled KdV Equations

In this section, the Hamiltonian formulations of the coupled KdV type equations, which are not in bi-Hamiltonian form, are solved by AVF method. These coupled equations are named as KdV-KdV and symmetric KdV-KdV systems in [8] because of the dispersive terms of third-order derivatives and model surface water waves with two variables u and v, where both propagates in time and space. In particular both of the coupled KdV-KdV systems are approximations to two dimensional Euler equations for surface wave propagation along a

horizontal channel with an ideal fluid inside. In the model of this ideal fluid, the independent space and time variable x and t represent the position and the elapsed time, respectively along the channel, where u is the horizontal velocity and v is the deviation of the free surface from its rest position [8, 9].

4.2.1 KdV-KdV System

The coupled system

$$\begin{aligned} u_t + uu_x + v_x + \tfrac{1}{6}v_{xxx} &= 0, \\ v_t + (uv)_x + u_x + \tfrac{1}{6}u_{xxx} &= 0 \end{aligned} \tag{4.40}$$

is given in [8] with the Hamiltonian functional

$$\mathcal{H} = \int \left(-v^2 - u^2 - u^2 v + \frac{1}{6}u_x^2 + + \frac{1}{6}v_x^2 \right) dx$$

and we determine the Hamiltonian operator as

$$\mathcal{J} = \begin{pmatrix} 0 & \frac{D}{2} \\ \frac{D}{2} & 0 \end{pmatrix},$$

by checking whether the system (4.40) satisfies (2.12) with this Hamiltonian formulation as follows

$$\begin{aligned} \frac{\delta \mathcal{H}}{\delta u} &= \frac{\partial H}{\partial u} - \partial_x \left(\frac{\partial H}{\partial u_x} \right) = -2u - 2uv - \frac{u_{xx}}{3}, \\ \frac{\delta \mathcal{H}}{\delta v} &= \frac{\partial H}{\partial v} - \partial_x \left(\frac{\partial H}{\partial v_x} \right) = -2v - u^2 - \frac{v_{xx}}{3}, \end{aligned}$$

then

$$\frac{\partial u}{\partial t} = \mathcal{J} \begin{pmatrix} \frac{\delta \mathcal{H}}{\delta u} \\ \frac{\delta \mathcal{H}}{\delta v} \end{pmatrix} = \begin{pmatrix} -uu_x - v_x - \frac{1}{6}v_{xxx} \\ -(uv)_x - u_x - \frac{1}{6}u_{xxx} \end{pmatrix}.$$

Then the semi-discrete Hamiltonian operator and functional are found as

$$\bar{J} = \frac{1}{4\Delta x} \begin{pmatrix} 0 & A \\ A & 0 \end{pmatrix}, \quad \bar{H} = \sum_{j=1}^{N} \left(-u_j^2 - v_j^2 - u_j^2 v_j + \frac{1}{6\Delta x^2}(u_{j+1} - u_j)^2 + \frac{1}{6\Delta x^2}(v_{j+1} - v_j)^2 \right) \Delta x$$

with the matrix A as in (4.3). The gradient of the semi-discrete Hamiltonian functional is obtained as

$$\nabla\bar{H}(u,v) = \begin{pmatrix} -2u_1 - 2u_1v_1 - \frac{1}{3\Delta x^2}(u_2 - 2u_1 + u_N) \\ \vdots \\ -2u_j - 2u_jv_j - \frac{1}{3\Delta x^2}\left(u_{j+1} - 2u_j + u_{j-1}\right) \\ \vdots \\ -2u_N - 2u_Nv_N - \frac{1}{3\Delta x^2}(u_1 - 2u_N + u_{N-1}) \\ -2v_1 - u_1^2 - \frac{1}{3\Delta x^2}(v_2 - 2v_1 + v_N) \\ \vdots \\ -2v_j - u_j^2 - \frac{1}{3\Delta x^2}\left(v_{j+1} - 2v_j + v_{j-1}\right) \\ \vdots \\ -2v_N - u_N^2 - \frac{1}{3\Delta x^2}(v_1 - 2v_N + v_{N-1}) \end{pmatrix},$$

where $j = 1, \ldots, N$. Then when we apply the AVF method, the resulting equations in the vector form are

$$\begin{aligned} \frac{u^{n+1} - u^n}{\Delta t} &= -\frac{1}{4\Delta x}A\left(v^n + \frac{1}{3}\hat{u}^n\right) - \frac{1}{24\Delta x^3}A\left(\tilde{v}^n + \tilde{v}^{n+1}\right), \\ \frac{v^{n+1} - v^n}{\Delta t} &= -\frac{1}{4\Delta x}A\left(u^n + \widetilde{uv}\right) - \frac{1}{24\Delta x^3}A\left(\tilde{u}^n + \tilde{u}^{n+1}\right), \end{aligned}$$

where the vectors u^n, v^n, $\tilde{u}^n$, $\tilde{v}^n$, $\hat{u}^n$ and $\widetilde{uv}$ are previously introduced.

The Jacobian is a $2N \times 2N$ dimensional block square matrix $\bar{J}_F(u^{n+1}, v^{n+1})$ such that

$$\bar{J}_F(u^{n+1}, v^{n+1}) = \left(\begin{array}{c|c} \bar{J}_{F1} & \bar{J}_{F2} \\ \hline \bar{J}_{F3} & \bar{J}_{F4} \end{array}\right),$$

with the matrices

$$\begin{aligned} \bar{J}_{F1} &= I + sAdiag(2u^{n+1}) + sAdiag(u^n), \\ \bar{J}_{F2} &= 3sA + rAP, \\ \bar{J}_{F3} &= sAdiag(2v^{n+1}) + sAdiag(v^n) + 3sA + rAP, \\ \bar{J}_{F4} &= I + sAdiag(2u^{n+1}) + sAdiag(u^n), \end{aligned}$$

where the constants are $r = \Delta t/24\Delta x^3$ and $r = \Delta t/12\Delta x$.

4.2.2 Symmetric KdV-KdV System

The coupled system of equations of the symmetric KdV-KdV are given in [9] without giving the Hamiltonian functional

$$\begin{aligned} u_t + \tfrac{3}{2}uu_x + \tfrac{1}{2}vv_x + v_x + \tfrac{1}{6}v_{xxx} &= 0, \\ v_t + \tfrac{1}{2}(uv)_x + u_x + \tfrac{1}{6}u_{xxx} &= 0. \end{aligned} \tag{4.41}$$

Introducing the Hamiltonian

$$\mathcal{H} = \int \left(-uv - \frac{1}{4}uv^2 - \frac{u^3}{4} - \frac{1}{6}uv_{xx} \right) dx,$$

which is configured from the Hamiltonian given in [26], is for the coupled system (4.41). Then the skew-adjoint operator is

$$\mathcal{J} = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}.$$

We obtain the coupled Hamiltonian system of equations (4.41) as

$$\begin{aligned} \frac{\delta \mathcal{H}}{\delta u} &= \frac{\partial H}{\partial u} - \partial_x \left(\frac{\partial H}{\partial u_x} \right) = -v - \frac{v^2}{4} - \frac{3}{4}u^2 - \frac{v_{xx}}{6}, \\ \frac{\delta \mathcal{H}}{\delta v} &= \frac{\partial H}{\partial v} - \partial_x \left(\frac{\partial H}{\partial v_x} \right) + \partial_x^2 \left(\frac{\partial H}{\partial v_{xx}} \right) = -u - \frac{uv}{2} - \frac{u_{xx}}{6}. \end{aligned}$$

The operator and the functional are written in the semi-discrete form as follows

$$\bar{J} = \frac{1}{2\Delta x} \begin{pmatrix} 0 & A \\ A & 0 \end{pmatrix}, \quad \bar{H} = \sum_{j=1}^{N} \left(-u_j v_j - \frac{u_j v_j^2}{4} - \frac{u_j^3}{4} - \frac{u_j (v_{j+1} - 2v_j + v_{j-1})}{6\Delta x^2} \right) \Delta x.$$

Then the gradient of the centrally discretized Hamiltonian functional becomes

$$\nabla \bar{H}(u, v) = \begin{pmatrix} -v_1 - \frac{v_1^2}{4} - \frac{3}{4}v_1^2 - \frac{1}{6\Delta x^2}(v_2 - 2v_1 + v_N) \\ \vdots \\ -v_j - \frac{v_j^2}{4} - \frac{3}{4}v_j^2 - \frac{1}{6\Delta x^2}\left(v_{j+1} - 2v_j + v_{j-1}\right) \\ \vdots \\ -v_N - \frac{v_N^2}{4} - \frac{3}{4}v_N^2 - \frac{1}{6\Delta x^2}(v_1 - 2v_N + v_{N-1}) \\ -u_1 - \frac{u_1 v_1}{2} - \frac{1}{6\Delta x^2}(u_2 - 2u_1 + u_{N-1}) \\ \vdots \\ -u_j - \frac{u_j v_j}{2} - \frac{1}{6\Delta x^2}\left(u_{j+1} - 2u_j + u_{j-1}\right) \\ \vdots \\ -u_N - \frac{u_N v_N}{2} - \frac{1}{6\Delta x^2}(u_1 - 2u_N + u_{N-1}) \end{pmatrix}$$

for $j = 1, \ldots, N$ and applying the AVF method leads to the following system of equations

$$\begin{aligned}
\frac{u^{n+1} - u^n}{\Delta t} &= -\frac{1}{4\Delta x} A \left(v^n + v^{n+1} \right) - \frac{1}{2\Delta x} A \left(\frac{1}{4} \hat{u} + \frac{1}{12} \hat{v} \right) - \frac{1}{12\Delta x^3} A \left(\tilde{v}^n + \tilde{v}^{n+1} \right), \\
\frac{v^{n+1} - v^n}{\Delta t} &= -\frac{1}{4\Delta x} A \left(u^n + u^{n+1} \right) - \frac{1}{8\Delta x} A \widetilde{uv} - \frac{1}{12\Delta x^3} A \left(\tilde{u}^n + \tilde{u}^{n+1} \right).
\end{aligned}$$

The square block Jacobian matrix is of the form 4.36, with the matrices

$$\begin{aligned}
\bar{J}_{F1} &= I + 3sAdiag(2u^{n+1}) + 3sAdiag(u^n), \\
\bar{J}_{F2} &= \bar{J}_{F3} = 6sA + sAdiag(2v^{n+1}) + sAdiag(v^n) + rAP, \\
\bar{J}_{F4} &= I + sAdiag(2u^{n+1}) + sAdiag(u^n),
\end{aligned}$$

with the constants are $r = \Delta t / 12\Delta x^3$ and $r = \Delta t / 24\Delta x$.

CHAPTER 5

NUMERICAL RESULTS

In this chapter, we will look at the performance of the AVF method for the KdV- type equations by looking the wave forms, the energy errors and the Casimirs. In all computations, energy error is defined as

$$Error = H - \bar{H},$$

where H is the exact energy and $\bar{H}$ is the discrete energy obtained by the AVF method. The error in the Casimirs can be defined analogously.

5.1 Korteweg de Vries Equation

The general form of the KdV equation is given as (2.14) with its bi-Hamiltonian formulations in the previous chapter. We solve the KdV equation, using the AVF method (3.12) with the initial condition

$$u(x, 0) = \cos(\pi x) \tag{5.1}$$

for the constants $\alpha = -1$, $\rho = 0$ and $\nu = -0.022^2$. The error in the semi-discretized energy $\bar{H}_2$ and in the discrete quadratic conserved quantity $\bar{I}_2 = \sum_{j=1}^{N} \frac{1}{2} u_j^2 \Delta x$, which was introduced in the example in the section 2.2 can be seen in Figure 5.1. The computations are done with respect to the first Hamiltonian pair of KdV equation $\mathcal{J}_1$ in (4.1) and $\mathcal{H}_2$ in (4.2). The trivial conserved quantity $\bar{I}_1 = \sum_{j=1}^{N} u_j \, \Delta x$ is not examined since the linear quantity is already conserved.

The error in the energy $\mathcal{H}_1$ of the second formulation $\mathcal{J}_2$, $\mathcal{H}_1$ is shown in Figure 5.2, but $\bar{I}_2 = \sum_{j=1}^{N} \frac{1}{2} u_j^2 \Delta x$ is not applicable as a conserved quantity since it is equal to the Hamiltonian

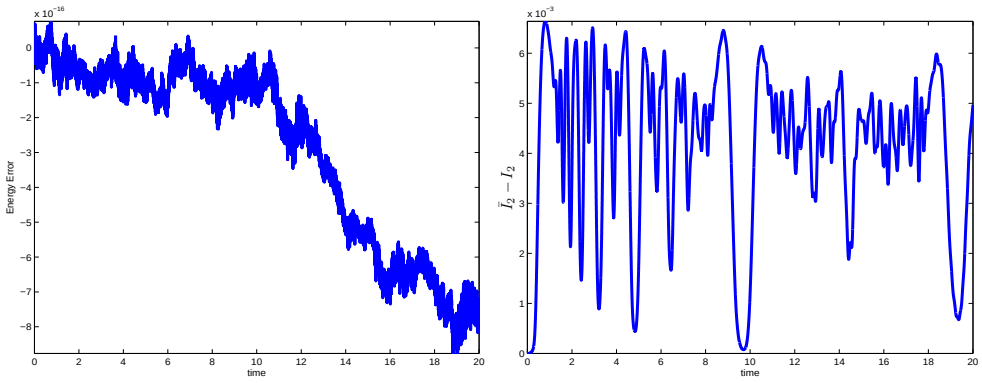


Figure 5.1: KdV equation: Energy error (left) and error for $\bar{I}_2$ (right) for the first formulation with $\Delta t = 0.001$ and $\Delta x = 0.01$ where $x \in [0, 2]$ of equally spaced with initial condition $\cos(\pi x)$ and constants $\alpha = -1, \rho = 0, \nu = -0.022^2$

of the second pair already.

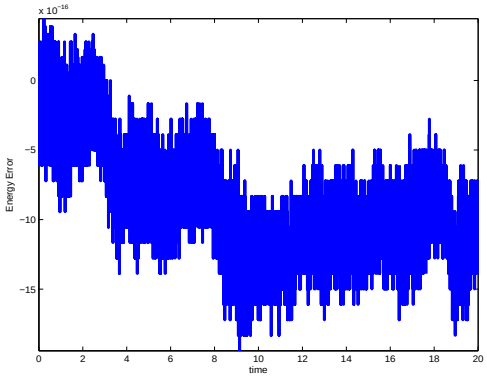


Figure 5.2: KdV equation: Energy error for the second formulation with $\Delta t = 0.001$ and $\Delta x = 0.01$ where $x \in [0, 2]$ of equally spaced with initial condition $\cos(\pi x)$ and constants $\alpha = -1, \rho = 0, \nu = -0.022^2$.

The solutions of the KdV equation using the AVF method can be compared with the symplectic and multisymplectic solutions obtained in [3] in Figure 5.3. The solutions display a similar profile at different times for the first Hamiltonian formulation, where the same result is also obtained for the second Hamiltonian pair.

When we solve the KdV equation for a smaller $\Delta x = 0.005$, the error in the energy at time $t = 5$ are $7.8e-18$ and $6.6e-16$, at $t = 10$ are $1.8e-16$ and $1.9e-15$ for the first and second Hamiltonian formulations, respectively. These results are considerably small compared to the errors obtained in [3] by using the multisymplectic, narrow box and the semi-explicit symplectic methods.

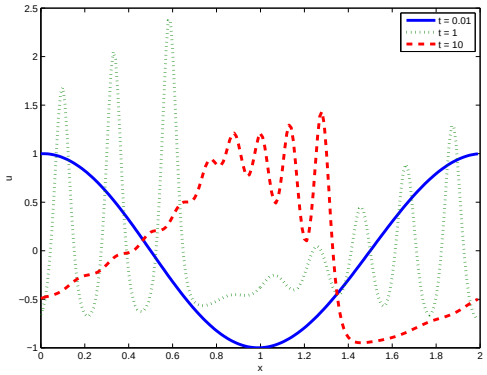


Figure 5.3: KdV equation: Solution for first formulation at various times $t = 0.01$, $t = 1$ and $t = 10$ obtained with same conditions as in Figure 5.1.

If we check the solution for a rough choice of $\Delta x = 0.02$, both of the Hamiltonian formulations give the same result as in Figure 5.4 at $t = 10$, which resembles the graphs obtained from the semi-explicit symplectic and the implicit midpoint methods in [3]. This is an expected result, since the AVF method has the same order as the semi-explicit symplectic and the implicit methods.

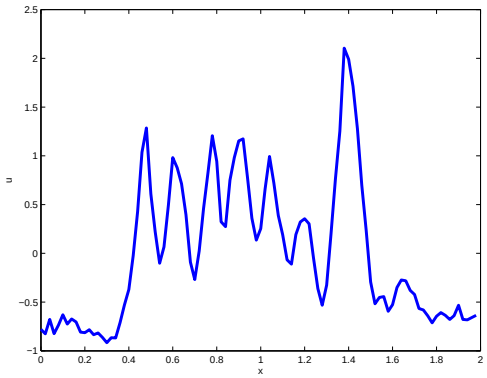


Figure 5.4: KdV equation: Solution for first formulation at $t = 10$ with $\Delta t = 0.004$ and $\Delta x = 0.02$ where $x \in [0, 2]$ of equally spaced with initial condition $\cos(\pi x)$ and constants $\alpha = -1, \rho = 0, \nu = -0.022^2$

For the first Hamiltonian formulation snapshots of the solution can be seen in Figure 5.5, where the second Hamiltonian formulation yield also consistent result with the Figure 2 in [64].

In [2], same periodic initial condition (5.1) is used for different constant values of $\alpha = -3/4$, $\rho = -1/10$ and $\nu = -0.002/3$. The errors in the energy and the quadratic conserved quantity

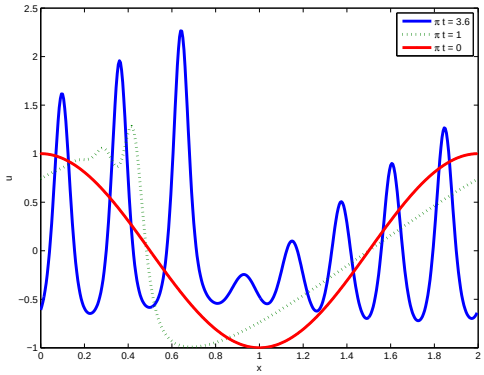


Figure 5.5: KdV equation: Solution for first formulation at various times $t = 0$, $t = 1/\pi$, $t = 3.6/\pi$ with $\Delta t = 5 \times 10^{-3}/\pi$ and $\Delta x = 0.001$ where $x \in [0, 2]$ of equally spaced with initial condition $\cos(\pi x)$ and constants $\alpha = -1$, $\rho = 0$, $\nu = -0.022^2$

for the first formulation are shown in Figure 5.6,where the error is of order 10^{-16}. The result obtained from the second formulation is same for the energy error. The error in the energy is around 10^{-3} in [2], therefore the results that we obtain using AVF methods are dramatically small when compared. The error in the Casimir quantity $\bar{I}_2 = \sum_{j=1}^{N} \frac{1}{2} u_j^2 \Delta x$ of the first formulation is also displayed in Figure 5.6, where the conservation is not in higher order as the Hamiltonian, however, it still shows conservation up to 10^{-3}.

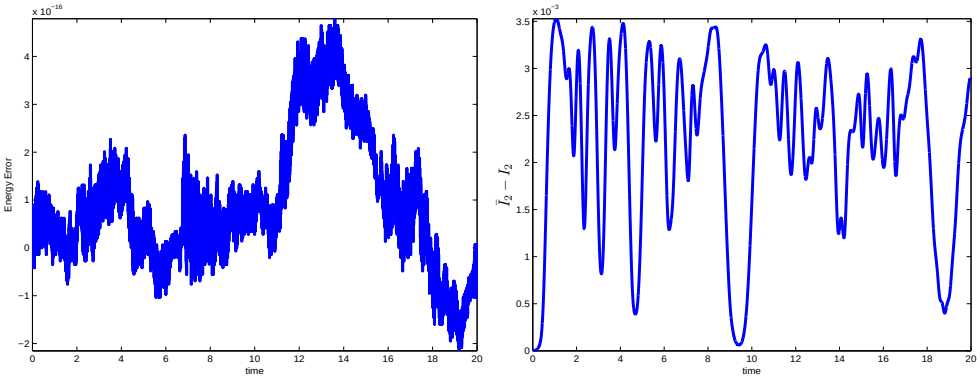


Figure 5.6: KdV equation: Energy error (left) and error for $\bar{I}_2$ (right) for the first formulation with $\Delta t = 0.001$ and $\Delta x = 0.01$ where $x \in [-1, 1]$ of equally spaced with initial condition $\cos(\pi x)$ and constants $\alpha = -3/4$, $\rho = -1/10$, $\nu = -0.002/3$.

Figure 5.7 shows the solution of the KdV equation using the AVF method for $t = 0, 1, 2, 3$ and 4.5. One can see that those solutions are agree with the solution in [2].

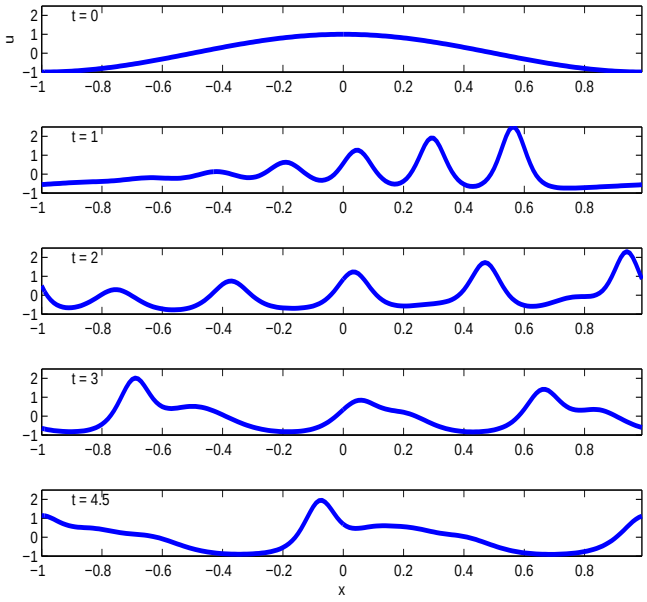


Figure 5.7: KdV equation: Snapshots of the solution for first formulation for $t = 0, 1, 2, 3$ and 4.5 obtained using the same conditions as in Figure 5.6

A different initial condition is proposed in [64] as

$$u(x, 0) = sech^2\left(\frac{x}{\sqrt{2}}\right) \tag{5.2}$$

with the constants $\alpha = -6$, $\rho = 0$ and $\nu = -1$. Using these, the computed error in the Hamiltonian and the Casimir quantity for the first formulation can be seen in Figure 5.8. Figure 5.8 shows that the energy is exactly preserved by the AVF method, whereas the Casimir is well preserved, whose order of error is 10^{-3}. The second formulation computations results are similar to those obtained from the first Hamiltonian formulation, where the error is of order 10^{-15} for energy. The single soliton solution is displayed in Figure 5.9, which is exactly same as the one given in [64].

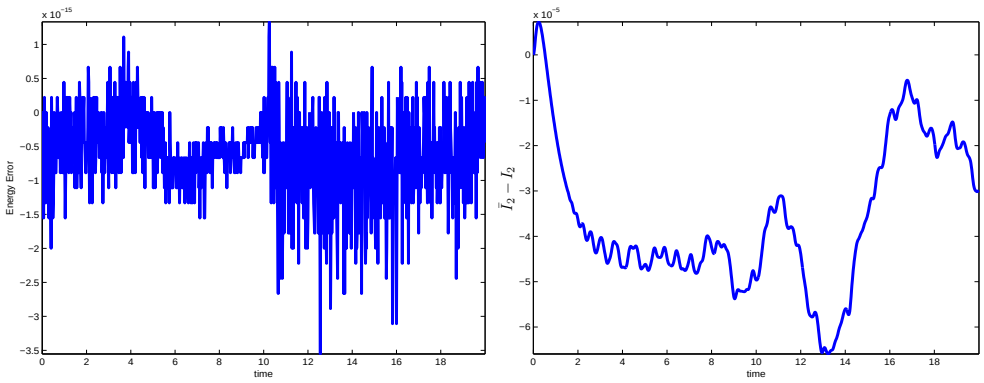


Figure 5.8: KdV equation: Energy error (left) and error for $\bar{I}_2$ (right) for the first formulation with $\Delta t = 0.02$ and $\Delta x = 40/150$ where $x \in [-20, 20]$ of equally spaced with initial condition $sech^2\left(\frac{x}{\sqrt{2}}\right)$ and constants $\alpha = -6$, $\rho = 0$, $\nu = -1$.

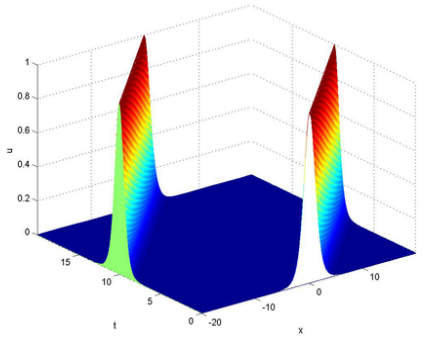


Figure 5.9: KdV equation: Single soliton for the first formulation obtained using the same conditions as in Figure 5.8.

The initial condition

$$u(x,0) = 6sech^2(x) \tag{5.3}$$

for the KdV equation without the term ρu_x, with constants of $\alpha = -6$ and $\nu = -1$ is used in [3, 64].

In [3], the solution is shown, which is obtained for the snapshots $t = 4$ and $t = 100$ using four different methods,that are, semi-explicit symplectic, multisymplectic, narrow box and implicit midpoint. The corresponding solution using AVF method can be seen in Figure 5.10. The results are given for the first Hamiltonian pair. The results for the second formulation is also similar. Those solutions are consistent with the results in [3] obtained by the implicit midpoint rule.

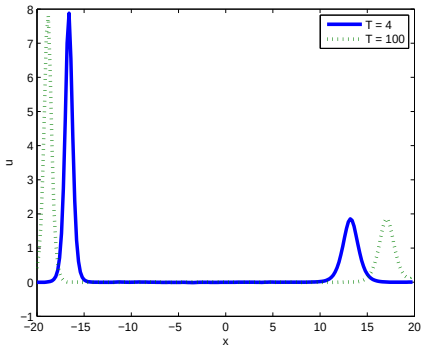


Figure 5.10: KdV equation: Solution for first formulation at various times $t = 4$, $t = 100$ with $\Delta t = 0.01$ and $\Delta x = 0.005$ where $x \in [-20, 20]$ of equally spaced with initial condition $6sech^2(x)$ and constants $\alpha = -6$, $\rho = 0$, $\nu = -1$

If Δx and Δt are taken smaller as $40/300$ and 0.002, respectively and the calculation is done for the time interval $[0, 4]$ with the initial condition (5.3), the temporal development of the solution in Figure 5.11 and the two soliton in Figure 5.12 are obtained, which give the opportunity to compare the results with the results in [64].

Figure 5.11 represents the collision of two solutions of the KdV equation (2.14) using the AVF method (3.12) with the initial condition (5.3) for $\Delta x = 40/300$ and $\Delta t = 0.002$ on the time interval $[0, 4]$. We see that two waves are initially located at $x = 0$ and the taller one travels faster than the shorter one. Both waves move to the right direction. The taller wave catches the shorter one approximately at time $t = 3.17$ and then continue to move to the right direction. In this collision we see that, waves keep their shapes.

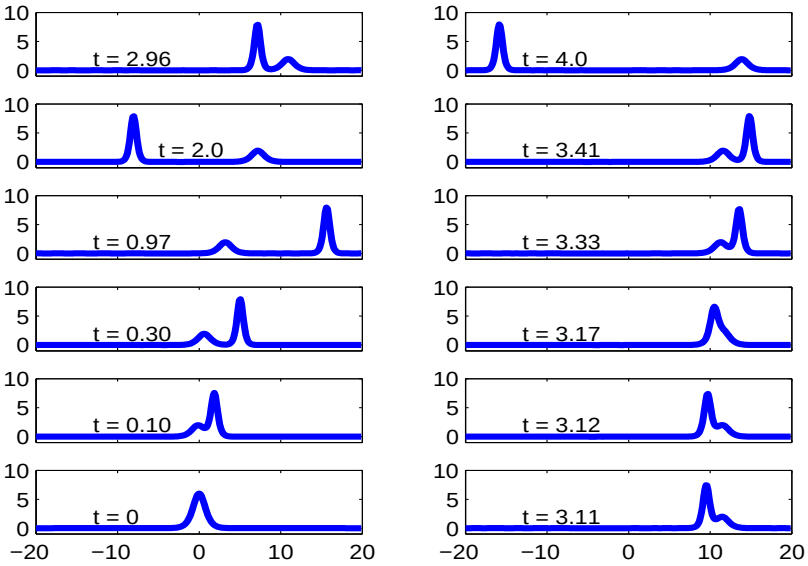


Figure 5.11: KdV equation: Solution for first formulation at various times for $t \in [0, 4]$ with $\Delta t = 0.002$ and $\Delta x = 40/300$ where $x \in [-20, 20]$ of equally spaced with initial condition $6sech^2(x)$ and constants $\alpha = -6$, $\rho = 0$, $\nu = -1$

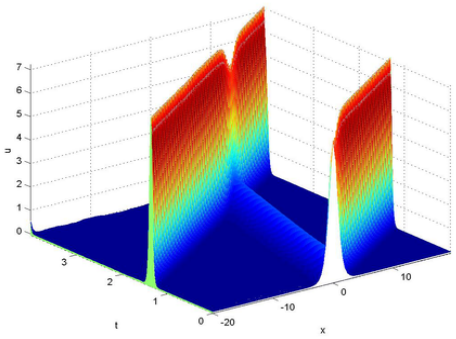


Figure 5.12: KdV equation: Two solitons for the first formulation using the same conditions as in Figure 5.11

Energy conservation of the waves can also be seen from the Figure 5.13, in which the error in the energies $\mathcal{H}_1, \mathcal{H}_2$ are approximately 10^{-12}.

When we take $\Delta x = 40/200$ and $\Delta t = 0.01$, the error in the energy with respect to the first and the second pairs of Hamiltonian are in Figure 5.13. The error at time $t = 4$ are $2.2e-13$ and $3.9e-14$; at $t = 100$ are $1.8e-11$ and $1.4e-12$ for the first and second pairs, respectively. Even if the computations are done for greater Δt values than used in [3], the results that we obtain are more efficient than [3]. In [3] the best approximation for the energy is correct of order 10^{-4}, but for our computations we get the error around 10^{-12}. These results clearly show that the conservation laws hold for the AVF method up to machine precision.

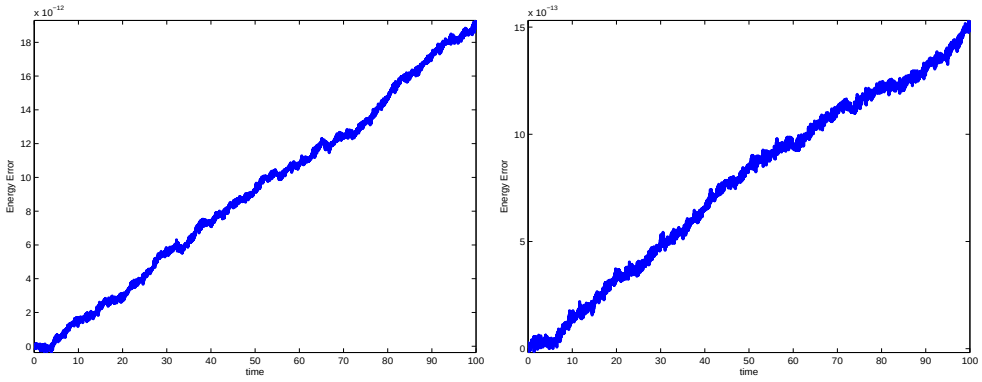


Figure 5.13: KdV equation: Energy error with respect to first(left) and second(right) formulations with $\Delta t = 0.01$ and $\Delta x = 0.005$ and the rest of the conditions are same as in Figure 5.11

5.2 Modified Korteweg de Vries Equation

For the modified KdV equation (4.20), many initial conditions exist and some of them are introduced in [19, 65].

A general solution offered for the mKdV equation in [65] is

$$u(x,t) = 2\eta sech 2\eta(x - 4\eta^2 t - x_0). \tag{5.4}$$

To have a one soliton solution, (5.4) is used as the initial condition, which is centrally located, that is $x_0 = 0$ with the constant $\eta = 1$ at $t = 0$. The error in the energy with respect to first and second formulations can be seen in Figure 5.14. The results again show the conservation of the energy within small error values with respect to both Hamiltonian formulations.

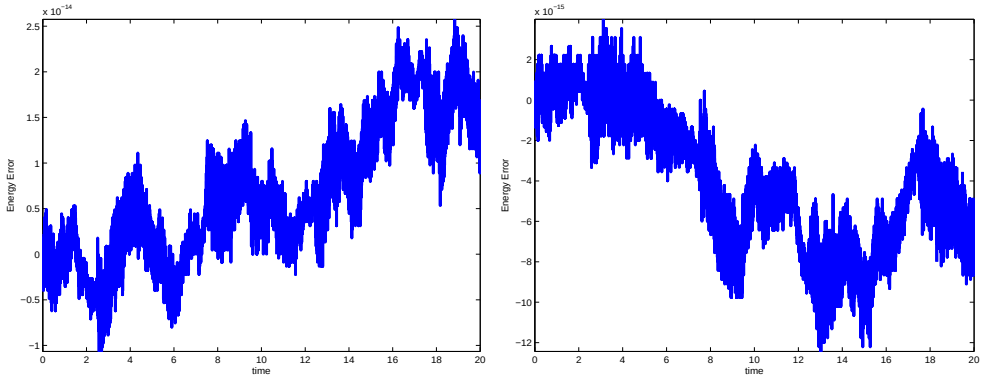


Figure 5.14: mKdV equation: Energy error with respect to first(left) and second(right) formulations with $\Delta t = 0.01$ and $\Delta x = 20/256$ where $x \in [-10, 10]$ of equally spaced with initial condition $2sech(2x)$ and constants $\alpha = 6, \beta = 1$.

The conserved quantity $\mathcal{I}_2$ is the same as the one for the KdV equation, which is $\mathcal{I}_2 = \frac{1}{2}\int u^2 dx$. This can be computed only for the first Hamiltonian formulation of mKdV equation, as for the second one $\mathcal{I}_2$ corresponds to the total energy itself. With respect to the first formulation the difference between the continuous and the discrete $\mathcal{I}_2$, which is represented as $\bar{I}_2$, can be seen in Figure 5.15 for long term propagation up to $t = 20$.

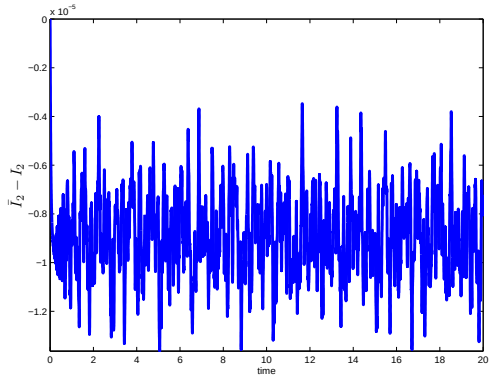


Figure 5.15: mKdV equation: Energy in $\mathcal{I}_2$ with respect to first formulation with the same conditions as in Figure 5.14

When the same conditions with the Figure 5.15 are used, one soliton for the mKdV is obtained as in Figure 5.16 with respect to second formulation, where the first one also gives the same result. When we compare the soliton figure with the original one soliton obtained from the dual-Petrov-Galerkin spectral method used in [65], the solution that we obtained seems to have two peaks and may seem as different at first instant. However, in [65] only the first group of waves is presented due to the homogenous boundary condition. The other groups of

waves in our case repeat itself since we use a periodic boundary condition.

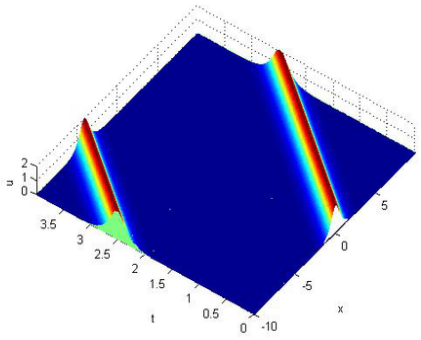


Figure 5.16: One soliton for mKdV equation for the first formulation using the same conditions as in Figure 5.14

Now, we will check the performance of the AVF method for interaction of the solitons. We use the initial condition

$$u(x,0) = \sum_{i=1}^{3} 2\eta_i sech 2\eta_i (x - x_i) \tag{5.5}$$

with

$$\eta_1 = 2, \quad \eta_2 = 1, \quad \eta_3 = 0.5,$$
$$x_1 = -10, \quad x_2 = 0, \quad x_3 = 10.$$

The initial condition (5.5) represents three solitons initially located as $x = -10, 0$ and 10.

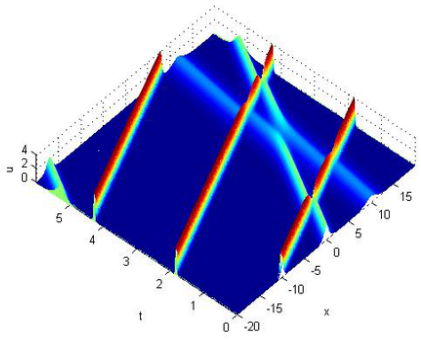


Figure 5.17: Interaction of three solitary waves for the first formulation using the initial condition obtained from (5.5) with $\Delta t = 0.0005$ and $\Delta x = 40/512$ where $x \in [-20, 20]$ of equally spaced

In Figure 5.17, we plot the time evolution of the solution of interaction of the solitons. The

moment of interaction can be clearly seen in the lightened region of the figure, where the waves collide and the phases are shifted. Within the collision, the velocities and the shapes of the group of waves are conserved. This is a consistent result with the idea of solitons, since solitons are the waves that have both wave and particle properties. Hence in the figure 5.17, as a result of the particle property of the solitons, the propagating waves are not destroyed in shape. The reason of having more than one peak in our interacting solitons, which is not the case in [65], but this again stems from the periodicity of the initial condition.

A different soliton solution can be obtained using a third initial condition. This is given in [54] as

$$u(x, 0) = \exp(-1.5x^2), \tag{5.6}$$

which is a Gaussian wave packet.

Using the time step of $\Delta t = 0.001$ for $t \in [0, 30]$ and $x \in [-20, 20]$ with $N = 512$ of equal spacing, the evolution of the wave packet is shown in Figure 5.18.

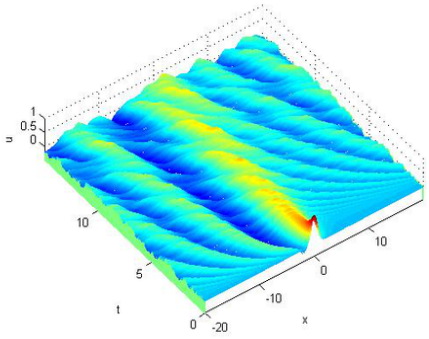


Figure 5.18: Solitary waves generated by an initial Gaussian wave for mKdV equation.

The Gaussian wave packet generates a series of solitons without any observable reflections. The dispersive properties of the mKdV equation can be observed with the oscillations around the initially located group of waves in Figure 5.18. In order to see the corresponding error in the energy with respect to both of the Hamiltonian pairs, we plot the energy errors in Figure 5.19 and the conserved quantities in Figure 5.20.

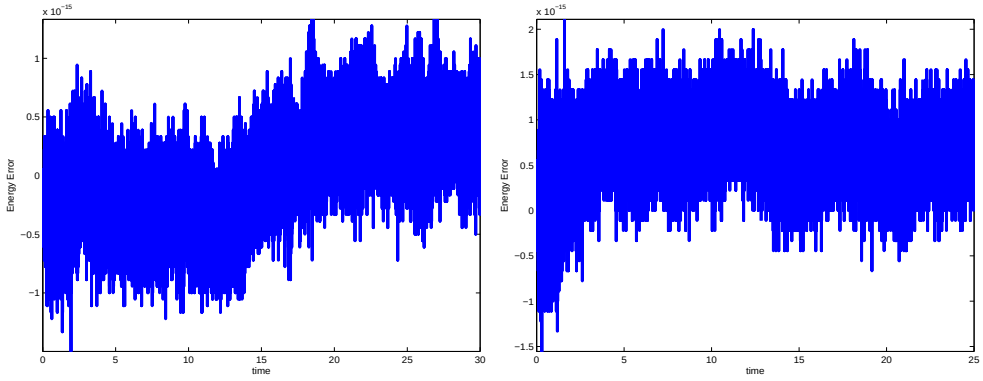


Figure 5.19: mKdV equation: Error in the energy of first (left) and second (right) formulations with $\Delta t = 0.001$ and $\Delta x = 40/512$ where $x \in [-20, 20]$ of equally spaced with initial condition $\exp(-1.5x^2)$ and constants $\alpha = 6, \beta = 1$

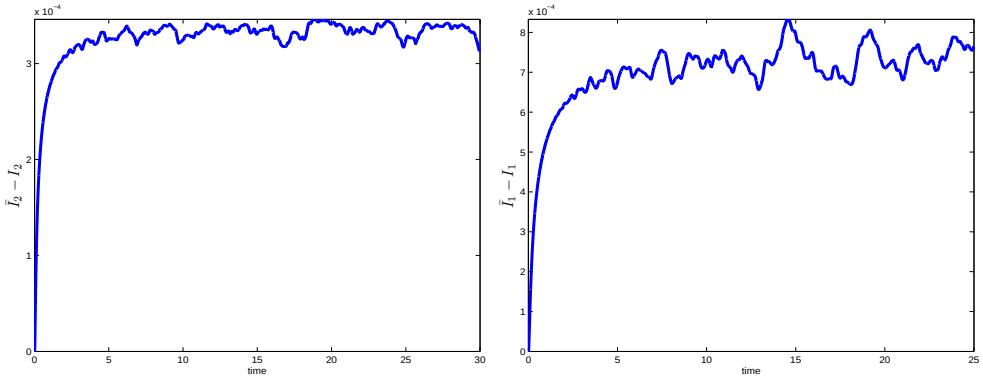


Figure 5.20: mKdV equation: Energy Casimir functions of the first $\mathcal{I}_2 = \int \frac{1}{2}u^2 dx$ (left) and second $\mathcal{I}_1 = \int u dx$ (right) Hamiltonian formulations with the same conditions as in Figure 5.19

5.3 Ito's System

Some numerical results are introduced in [61], where two different initial conditions are proposed.

The first initial condition is

$$u(x, 0) = \cos x, \quad v(x, 0) = \cos x, \tag{5.7}$$

which are clearly periodic. The computations are done using $N = 80$ cells for the equally spaced interval $[0, 2\pi]$. The error in the energies for the AVF method of two systems for long time propagation can be seen in Figure 5.21. The figure shows that the energies are preserved with respect to both formulations as expected up to the tolerance of the machine precision.

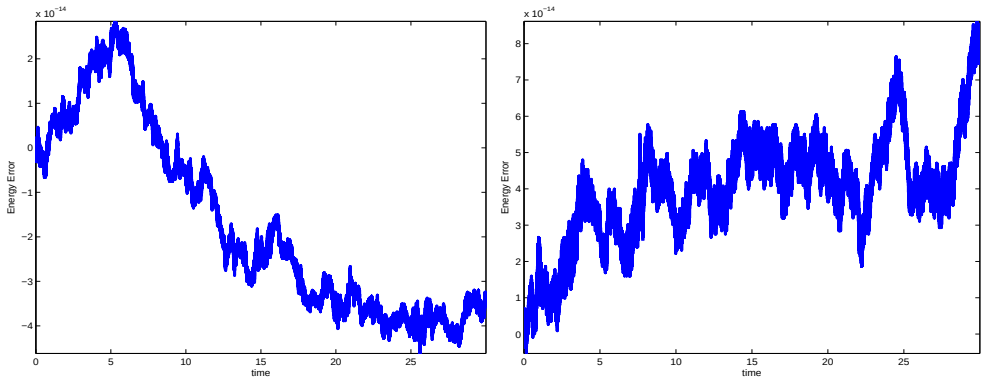


Figure 5.21: Ito's system: The error in the energy with respect to first (left) and the second (right) formulations with $\Delta t = 0.0001$ and $\Delta x = 2\pi/80$ where $x \in [0, 2\pi]$ of equally spaced with initial condition (5.7)

The infinitely many conserved quantities of the Ito's system of equations are investigated in [22]. Among these conserved quantities, when the, which is the linear sum of the variables such as $\mathcal{I}_1 = \int (u + v)\, dx$, is taken into consideration, the differences between the exact and the approximate conserved quantity with respect to both of the Hamiltonian formulations are displayed in Figure 5.22.

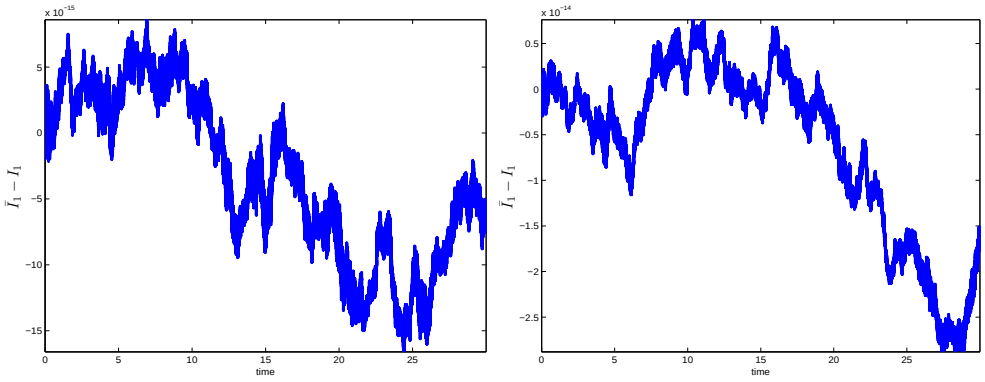


Figure 5.22: Ito's system: The error in the conserved quantity $\mathcal{I}_1$ for the first (left) and the second (right) formulations using the same conditions as in Figure 5.21

Also the snapshots of the solutions u and v at various times are displayed in Figures 5.23 and 5.24. The solutions found for instantaneous time levels shown here are obtained using the second formulation, however, the results obtained from the first formulation match up with the second one. In addition to the consistency of the results between the first and the second Hamiltonian formulations, they are same with the numerical results in [61], which were obtained by applying the local discontinuous Galerkin methods.

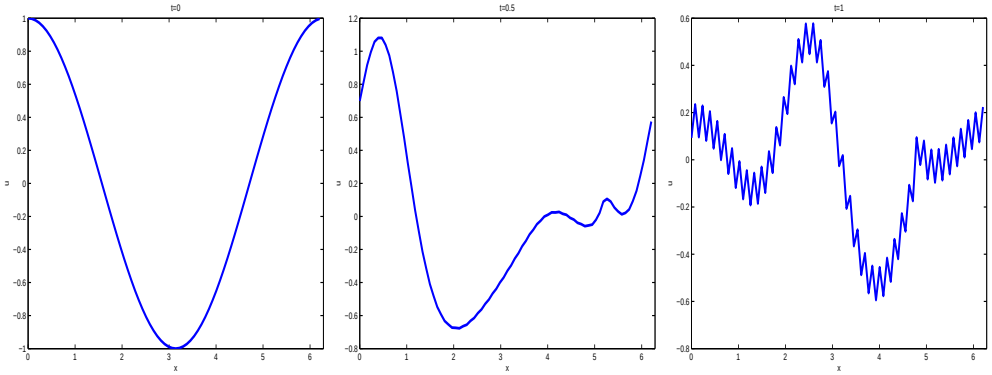


Figure 5.23: Solutions for u at time $t = 0, 0.5, 1$ from left to right using the same conditions as in Figure 5.21

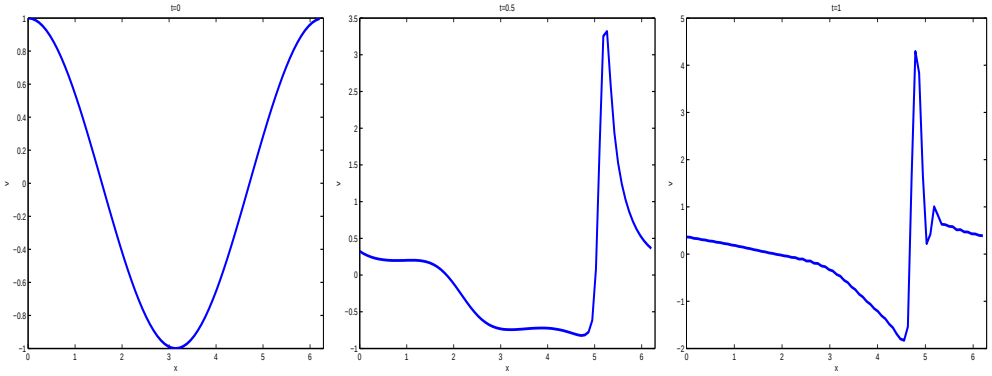


Figure 5.24: Solutions for v at time $t = 0, 0.5, 1$ from left to right using the same conditions as in Figure 5.21

Using a different initial condition, which is again given in [61] as

$$u(x, 0) = \exp(-x^2), \quad v(x, 0) = \exp(-x^2), \tag{5.8}$$

we can observe the energy preservation of AVF method in Figure 5.25. The results show that the difference between the exact and the approximated Hamiltonian functionals with respect to the bi-Hamiltonian formulation are considerably small and hence consistent with the assumption again that the energy is preserved up to the machine precision for the long time propagation of the wave.

In addition to the energy preservation, the preservation of the Casimir functional is displayed in the following Figure 5.26.

Similar to the results obtained for the first initial condition (5.7), solutions of the Ito's system for $t \in [0, 2]$ and some instantaneous solutions at $t = 0, 1$ and 2 can be seen in Figures 5.27

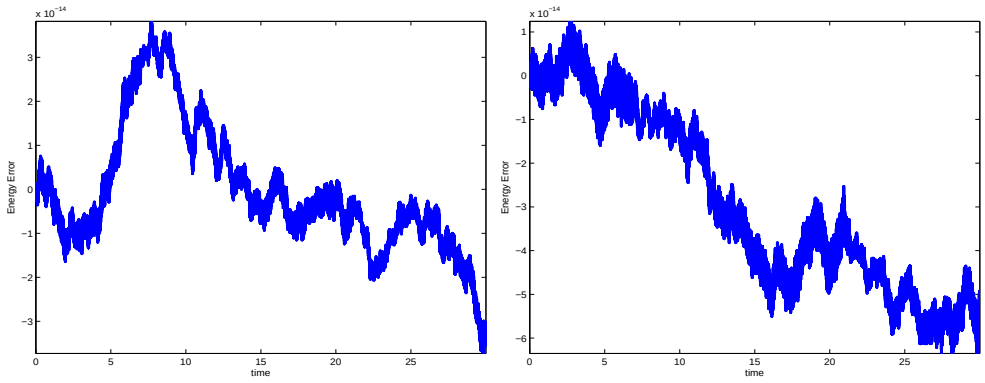


Figure 5.25: Ito's system: The error in the energy with respect to first (left) and the second (right) formulations with $\Delta t = 0.0001$ and $\Delta x = 30/160$ where $x \in [-15, 15]$ of equally spaced with initial condition (5.8)

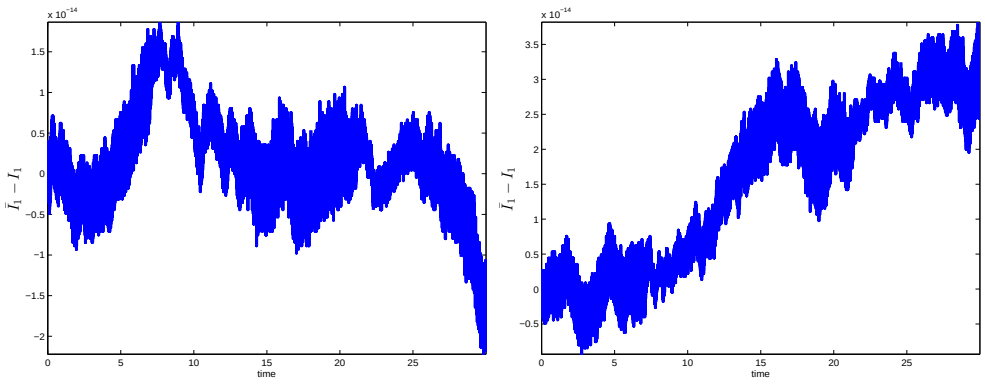


Figure 5.26: Ito's system: The error in the conserved quantity $\mathcal{I}_1$ for the first (left) and the second (right) formulations with $\Delta t = 0.0001$ and $\Delta x = 30/160$ where $x \in [-15, 15]$ of equally spaced with initial condition (5.8)

and 5.28 for the variables u and v. The results are obtained using equally spaced interval of $x \in [-15, 15]$ using number of meshes $N = 160$ in space.

We note that the first equation of the Ito's system (4.33) is dispersive by looking the oscillations around the solution u in Figure 5.27, but the second equation (4.34) is not. Dispersive properties of the waves can be seen from the Figure 5.23 through Figure 5.28. The observed dispersion in the Figure 5.27 can be explained with a detailed dispersion analysis.

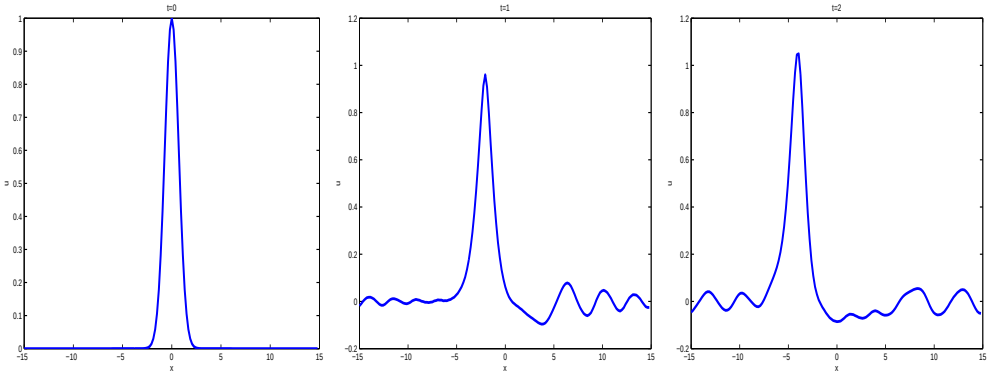


Figure 5.27: Solutions for u at various times using the same conditions as in Figure 5.25

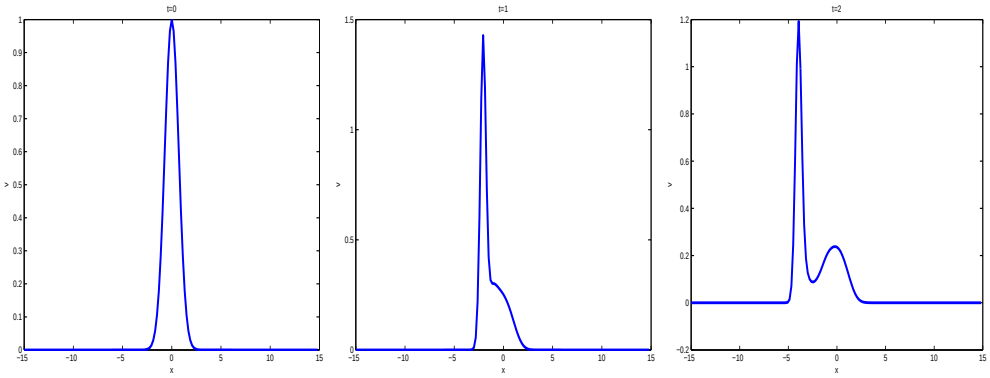


Figure 5.28: Solutions for v at various times using the same conditions as in Figure 5.25

5.4 KdV-KdV and Symmetric KdV-KdV Systems

The Hamiltonian formulations of the KdV-KdV system (4.40) and the symmetric KdV-KdV system (4.41) are studied in the previous chapter. The systems are solved using those formulations together with the periodic initial condition provided in [9], where the initial condition is generated by a Gaussian initial surface elevation profile and zero initial velocity as follows

$$u(x,0) = 0, \quad v(x,0) = 0.3\exp\left(-(x+100)^2/25\right). \tag{5.9}$$

The computations are done for the interval $x \in [-150, 150]$ and $N = 500$ equally spaced grids with the time step $\Delta t = 0.04$ up to $t = 100$. The error in the Hamiltonian functional are shown for both of the KdV-KdV systems in Figure 5.29. The figure shows that the energies in both systems are conserved up to 14 digits, up to $t = 100$, which shows the long time consistent behavior of the systems in energy.

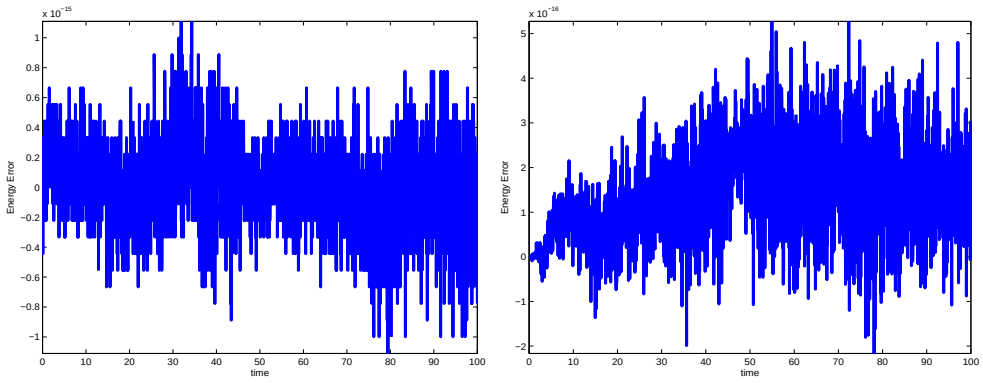


Figure 5.29: Error for the energy of the KdV-KdV and the symmetric KdV-KdV systems

Other invariant quantities rather than the energy of the KdV-KdV systems are introduced in [9]. For the KdV-KdV system, the conserved quantity is $\mathcal{I}_1 = \int uv\,dx$, whereas the symmetric system has the quantity $\mathcal{I}_1 = \int \left(u^2 + v^2\right) dx$. The conserved quantities for each of the KdV-KdV systems can be seen in Figure 5.30.

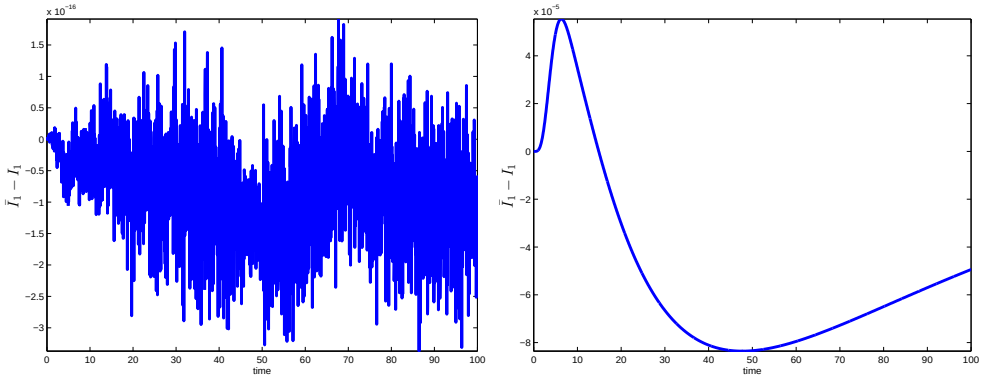


Figure 5.30: Conserved quantities $\mathcal{I}_1$ of the KdV-KdV (left) and the symmetric KdV-KdV system

We also examine the wave solutions for both of the systems. Since the results of the systems are similar, we only show the solution of the KdV-KdV system for the variables u and v in Figure 5.31.

In this section, the KdV-KdV and the symmetric KdV-KdV systems are investigated together using the same initial condition, since each system yield the same result when the waves are solved.

According to the figures and the results throughout this chapter, the solutions show that our

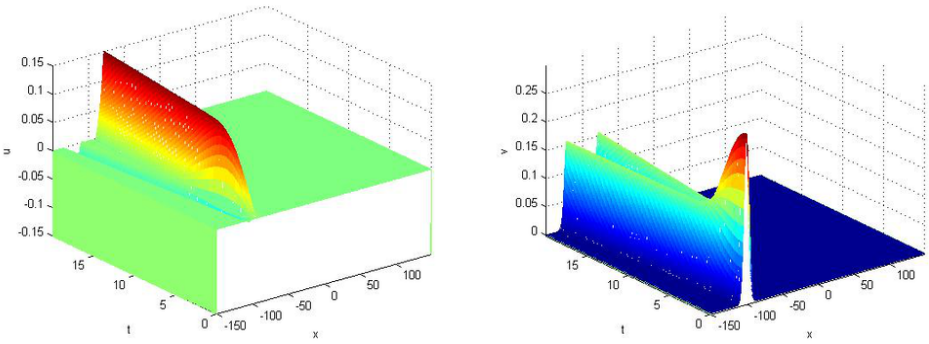


Figure 5.31: Solutions of the KdV-KdV systems for u (left) and v (right)

formulation gives consistent results with those in the articles. In addition to the wave forms, we see that the energy of the system and the Casimir functions are well preserved for the AVF method.

CHAPTER 6

DISPERSION ANALYSIS

Up to this chapter, the AVF method has been presented with the energy preservation property to determine the dynamics of the previously analyzed KdV-type equations.The problems involved are nonlinear like KdV-type equations, there are still many questions behind the behavior of the equations such that the magnitude of the global errors may be dependent with the local errors of the solution and the stability of the boundary conditions may be related with numerical dispersion. Conservation of energy does not give sufficient information about the behavior of the solutions. To understand the solution behavior of the AVF methods, we will consider the linearized equations and investigate numerical dispersion relations. The linearized PDEs will be solved again using the energy preserving AVF method in order to compare the continuous and the discrete versions of the dispersion relations of the equations. Investigation of the discrete dispersion relation plays an important role [1] together with the group velocity for the discretized linear and nonlinear wave equations.

The solutions of KdV type equations are in form of wave packets which are changing both in time and space. Wave packets are known as superposition of waves having different wave numbers. As the equations possess the wave nature, a general type of a proposed solution is symbolized with a wave number k and a frequency ω. Wave number and frequency are related concepts for the waves with the wavelength which is the distance between two consecutive points with equal phase on the wave in space. The relation between the wave number and the frequency of the superposed modes can be determined with the continuous dispersion relation. The dispersion for the waves can be defined as when the modes of differing wave numbers propagate at different speeds and that leads to some undesired oscillations in the solutions.

The dispersion can be defined as function of k as

$$\omega = \omega(k). \tag{6.1}$$

Throughout the chapter, the dispersion relations are analyzed for the continuous and the discretized linearized PDEs.

6.1 Linear Dispersion Relations

The solution of a linear problem with periodic initial condition may be obtained using the Fourier integral transform method which corresponds to the integral superposition of the normal mode solutions of the equation. The general normal mode solution of any linear time-dependent PDE with constant coefficients on an unbounded space domain is of the form

$$u(x,t) = \int_{-\infty}^{\infty} A(k)\, e^{ikx+\lambda(k)t}\, dk, \tag{6.2}$$

where $A(k)$ is an arbitrary function and i is imaginary unit.

Assuming each wave mode as a solution of a linearized PDE, the solution takes the form

$$u(x,t) = \hat{u}\, e^{ikx+\lambda(k)t}, \tag{6.3}$$

where $\hat{u}$ is constant and $\lambda(k)$ is a complex function which has to be chosen such that the exponential function satisfies the linearized equation. Then equation (6.3) can be explicitly written as

$$u(x,t) = \hat{u}\, e^{i(kx+Im[\lambda(k)]t)} e^{Re[\lambda(k)]t}. \tag{6.4}$$

If $Re(\lambda(k)) = 0$ for $\forall k$, then the equation is said to be conservative type and

$$\lambda(k) = i\omega(k),$$

where $\omega(k)$ is real valued $\forall k \in (-\infty, \infty)$, so the normal mode solutions as proposed in [52, 53] is of the form

$$u(x,t) = \hat{u}e^{i(kx+\omega(k)t)}. \tag{6.5}$$

In the following equations we give examples of some PDEs to explain the continuous dispersion relations.

Linear heat or diffusion equation : The equation

$$u_t = a^2 u_{xx} \tag{6.6}$$

is linear, therefore using the normal mode solutions (6.3) we can find the relation

$$\lambda(k) = -a^2 k^2.$$

As the equation for $\lambda(k)$ is real, the equation (6.6) is not conservative type, so it can not be dispersive.

Wave equation : The original PDE is

$$u_{tt} = a^2 u_{xx}. \tag{6.7}$$

The proposed normal mode solutions (6.3) for the linear equation (6.7) yield the relation

$$\lambda(k) = \pm iak.$$

The wave equation (6.7) is said to be conservative type, since $Re\lambda(k) = 0$ for all k values. This leads to the following dispersion relation

$$\omega(k) = ak,$$

which is dependent on k of order one. Therefore, the equation (6.7) is not dispersive.

The last equation is an example of both conservative and dispersive type.

The linear Klein-Gordon equation :

$$u_{tt} = a^2 u_{xx} - b^2 u. \tag{6.8}$$

Normal mode solutions (6.3) yield the equation

$$\lambda(k) = \pm i\sqrt{a^2 k^2 + b^2}. \tag{6.9}$$

Since the equation (6.9) has zero real part, the equation (6.8) is conservative type and it can be also concluded that the Klein-Gordon equation is dispersive with the dispersion relation

$$\omega(k) = \sqrt{a^2 k^2 + b^2}.$$

In addition to the dispersion relation, we need some more definitions about the speed of the waves. The phase velocity tells the propagation of speed of the wave front, where the term

$$\theta = kx - \omega(k)t$$

is called phase and

$$c(k) := \frac{\omega(k)}{k} \tag{6.10}$$

is called the phase velocity.

The group velocity $C(k)$ which characterizes the average speed of propagation of the composite wave package, can be found by differentiating the dispersion relation as

$$C(k) := \frac{d\omega(k)}{dk}. \tag{6.11}$$

For a PDE to be nondispersive, the phase velocity (6.10) should not depend on the wave number linearly, which shows different waves travel at the same speed. For example, if the dispersion relation is

$$\omega(k) = mk, \quad \text{where} \quad m \in \mathbb{R}$$

then the phase velocity $c(k) = m$ in (6.10) is clearly constant and the solution will be a function of $x - mt$ only, which is a wave traveling with speed m. Nevertheless, if the dispersion relation is not linear in k, then the system is called dispersive. That is, for the linear equation to be dispersive, the condition

$$\omega''(k) \neq 0$$

has to be satisfied and hence for different wave numbers k, each wave travels with different velocity. That means the nondispersive solutions have a traveling wave form, but a dispersive wave does not, since its component modes travel at different velocities. Therefore, the group velocity is more important than the phase velocity in order to characterize the wave behavior.

There is another important property of PDEs, which is numerical dissipation [56]. The partial differential equations conserves the energy, however, the discrete model may loose energy as time passes. This lost in energy may seem as a bad characteristic at first instant for some cases, however, in this way stability is provided and undesired oscillations are prevented. To check the dissipation, we need a general definition [56]:

Definition 6.1 *Let (6.5) be the solution of a linearized PDE with a dispersion relation (6.1). Since the wave number k has to be real, the absolute value of the wave is*

$$|e^{i(kx+\omega(k)t)}| = e^{-tIm\,\omega}.$$

If $Im\,\omega > 0$*, then the wave is said to be* ***dissipative****,* $\forall k \neq 0$ *and* ***nondissipative*** *if* $Im\,\omega = 0$.

This definition also shows that there are finite difference formulas that can be neither dissipative nor nondissipative. Whether a PDE is dissipative or nondissipative, it can be checked by looking at the PDE. If the differential equation contains only even ordered x derivatives, then the PDE is dissipative [55]. The dissipation is a result of decay or grow of the Fourier mode solutions. So, for an equation to be nondissipative, we need that the Fourier modes neither grow nor decay in time, which is possible only when the frequency ω is purely imaginary, that follows $\lambda(k)$ is real and the Fourier mode solution becomes $\hat{u}e^{ikx}e^{-\omega(k)t}$. Hence, the solution decay or grow depending on the sign of the frequency, which leads to dissipation. For our case, as the frequency ω is real, all KdV type equations considered in this thesis are nondissipative.

Now let us continue with the linearized equations to explore the dispersion relations of the form (6.1).

6.1.1 KdV-type Equations

6.1.1.1 KdV Equation

Assume that $\tilde{u} : \mathbb{R}^2 \to \mathbb{R}$ is a third order continuously differentiable function, such that $|\tilde{u}(x,t)| \ll 1$. Let also $u = \bar{u} + \tilde{u}$, where u and $\bar{u}$ are solutions to (2.14). Hence, $u_t = \bar{u}_t + \tilde{u}_t$, $u_x = \bar{u}_x + \tilde{u}_x$ and $u_{xxx} = \bar{u}_{xxx} + \tilde{u}_{xxx}$. Substituting into the equation (2.14), we get

$$\bar{u}_t + \tilde{u}_t = \alpha(\bar{u}\bar{u}_x + \bar{u}\tilde{u}_x + \tilde{u}\bar{u}_x + \tilde{u}\tilde{u}_x) + \rho(\bar{u}_x + \tilde{u}_x) + \nu(\bar{u}_{xxx} + \tilde{u}_{xxx}). \tag{6.12}$$

Rewriting (6.12) yields

$$\bar{u}_t + \tilde{u}_t = \alpha\bar{u}\bar{u}_x + \rho\bar{u}_x + \nu\bar{u}_{xxx} + \alpha\left(\bar{u}\tilde{u}_x + \tilde{u}\bar{u}_x + \tilde{u}\tilde{u}_x\right) + \rho\tilde{u}_x + \nu\tilde{u}_{xxx}. \tag{6.13}$$

Since $\bar{u}$ is the solution of (2.14)

$$\bar{u}_t - \alpha\bar{u}\bar{u}_x - \rho\bar{u}_x - \nu\bar{u}_{xxx} = 0.$$

Ignoring the quadratic term $\tilde{u}\tilde{u}_x$ in the equation (6.13) and assuming that the solution $\bar{u}$ is constant, that leads to $\bar{u}_x = 0$, then we get

$$\tilde{u}_t = \alpha_1\tilde{u}_x + \rho\tilde{u}_x + \nu\tilde{u}_{xxx}, \tag{6.14}$$

where $\alpha_1 = \alpha u_1$ is a constant. Then (6.14) is the linearized equation of the KdV equation (2.14) around the constant solution, $\bar{u}$.

The linearized equation admits the solution of the form (6.5), clearly $\tilde{u}_x = ik\hat{u}e^{i\omega t}e^{ikx} = ik\tilde{u}$, $\tilde{u}_{xxx} = -ik^3\tilde{u}$ and $\tilde{u}_t = i\omega\tilde{u}$. Substituting these into (6.14) and simplifying, we obtain the exact dispersion relation

$$\omega = \alpha_1 k + \rho k - \nu k^3 \tag{6.15}$$

of linearized KdV equation (6.14).

In addition to the dispersion relation, we can find the general phase velocity as

$$\frac{\omega}{k} = \alpha_1 + \rho - \nu k^2,$$

which is not linear in k, so the equation (6.14) is dispersive. The group velocity of the linearized equation (6.15) is

$$\frac{d\omega}{dk} = \alpha_1 + \rho - 3\nu k^2. \tag{6.16}$$

6.1.1.2 mKdV Equation

Using the same method as in the previous section, assume again that $\tilde{u} : \mathbb{R}^2 \to \mathbb{R}$ is a third order continuously differentiable function, such that $|\tilde{u}(x,t)| \ll 1$. When the solution of the form $u = \bar{u} + \tilde{u}$ is substituted into the equation (4.20), we obtain

$$\bar{u}_t + \tilde{u}_t = -\alpha(\bar{u}\bar{u}_x)^2(\bar{u}_x\tilde{u}_x) - \beta(\bar{u}_{xxx} + \tilde{u}_{xxx}). \tag{6.17}$$

Since we linearize the equation around constant solutions $\bar{u}$, they satisfy the following equation

$$\bar{u}_t + \alpha\bar{u}^2\bar{u}_x + \beta\bar{u}_{xxx}.$$

When we also ignore the higher order terms, the equation

$$\bar{u}_t + \tilde{u}_t = -\alpha\left(\bar{u}^2\bar{u}_x + 2\bar{u}\tilde{u}\bar{u}_x + \tilde{u}^2\bar{u}_x\right) - \alpha\left(\bar{u}^2\tilde{u}_x + 2\bar{u}\tilde{u}\tilde{u}_x + \tilde{u}^2\tilde{u}_x\right) - \beta\left(\bar{u}_{xxx} + \tilde{u}_{xxx}\right)$$

becomes

$$\tilde{u}_t = -\alpha(\bar{u}^2\tilde{u}_x - \tilde{u}\bar{u}\bar{u}_x) - \nu\tilde{u}_{xxx}. \tag{6.18}$$

As we linearize the equation (4.20) around constant solutions, the final linearized mKdV equation is

$$\tilde{u}_t = -a\tilde{u}_x - \nu\tilde{u}_{xxx}, \tag{6.19}$$

where $a = \alpha\bar{u}^2$. Substituting (6.5) into the linearized mKdV equation (6.19), we get the dispersion relation

$$\omega = -ak + \nu k^3. \tag{6.20}$$

The phase velocity (6.10) can then be computed as

$$\frac{\omega}{k} = -a + \nu k^2.$$

The continuous group velocity

$$\frac{d\omega}{dk} = -a + 3\nu\bar{k}^2$$

is obtained by the first derivative of the dispersion relation (6.20).

6.1.2 Coupled KdV-type Equations

In the following two sections the dispersion relation of the coupled systems are analyzed. As they are systems in two variable, their linearization has to be done in vector form.

6.1.2.1 Ito's System

The Ito's system (4.33) and (4.34) can be rewritten as

$$\begin{aligned} u_t - u_{xxx} - 6uu_x - 2vv_x &= 0 \\ v_t - 2uv_x - 2vu_x &= 0 \end{aligned} \tag{6.21}$$

and in vector form

$$y_t + By_{xxx} - A(u,v)y_x = 0 \tag{6.22}$$

with $y = (u,v)^T$,

$$B = \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad A = \begin{pmatrix} 6u & 2v \\ 2v & 2u \end{pmatrix}.$$

The equation (6.22) is linearized again around a constant solution $\bar{y} = (\bar{u},\bar{v})^T$ with a small perturbation of $\tilde{y} = (\tilde{u},\tilde{v})^T$ to y which gives $y = \bar{y} + \tilde{y}$, where $\tilde{y} : \left(\mathbb{R}^2 \times \mathbb{R}^2\right) \to (\mathbb{R} \times \mathbb{R})$ is composed from the third order continuously differentiable functions $\tilde{u}$ and $\tilde{v}$. As in the case of the KdV and the modified KdV equations in sections 6.1.1.1 and 6.1.1.2, respectively,

taking the derivatives, substituting them into (6.22), ignoring the higher order terms in $\tilde{y}$ and eliminating the derivatives of the constant solutions $\bar{y} = (\bar{u}, \bar{v})^T$ yields the equation

$$\tilde{y}_t + B\tilde{y}_{xxx} - A(\bar{u}, \bar{v})\tilde{y}_x = 0. \tag{6.23}$$

To get the dispersion relation, the spectral decomposition of the matrix $A(\bar{y})$ is introduced as in [5]. Following [5], we can write the matrix A in (6.23), $A = VDV^{-1}$ where D is the diagonal matrix with eigenvalues

$$\lambda_{1,2} = 4\bar{u} \pm 2\sqrt{\bar{u}^2 + \bar{v}^2} \tag{6.24}$$

on the diagonals and V is constructed by the eigenvectors of A on its columns. With the assumption of the eigenvalues to be equal, take $\lambda_1 = \lambda_2$ as constant and equal to a. Then assume that the multiplication of the matrices B and V is constant, so the linearized system of equations will be of the form

$$\tilde{u}_t = \tilde{u}_{xxx} + a\tilde{u}_x, \quad \tilde{v}_t = a\tilde{v}_x, \tag{6.25}$$

and the corresponding dispersion relations are

$$\omega_1 = -k^3 + ak, \quad \omega_2 = ak. \tag{6.26}$$

The phase velocities can be computed from the continuous dispersion relations (6.26) , which are

$$\frac{\omega_1}{k} = -k^2 + a, \quad \frac{\omega_2}{k} = a.$$

Since the phase velocity $\omega_2(k)$ has the property of $\omega_2''(k) = 0$, v is not a dispersive wave, whereas the solution u is dispersive.

The continuous group velocities of (6.25) are

$$\frac{d\omega_1}{dk} = -3k^2 + a, \quad \frac{d\omega_2}{dk} = a. \tag{6.27}$$

6.1.2.2 KdV-KdV System

The coupled system (4.40) is

$$\begin{aligned} &u_t + \tfrac{1}{6}v_{xxx} + uu_x + v_x = 0, \\ &v_t + \tfrac{1}{6}u_{xxx} + (1+v)u_x + uv_x = 0 \end{aligned} \tag{6.28}$$

and in vector form

$$y_t + \frac{1}{6}By_{xxx} + A(u,v)y_x = 0 \tag{6.29}$$

with $y = (u,v)^T$,

$$B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{6.30}$$

and

$$A(u,v) = \begin{pmatrix} u & 1 \\ v+1 & u \end{pmatrix}.$$

Similar to (6.22), (6.29) is linearized around the constant solution $\bar{y} = (\bar{u},\bar{v})^T$ with a small perturbation of $\tilde{y} = (\tilde{u},\tilde{v})^T$. When we substitute $y = \bar{y} + \tilde{y}$, $y_t = \bar{y}_t + \tilde{y}_t$, $y_x = \bar{y}_x + \tilde{y}_x$ and $y_{xxx} = \bar{y}_{xxx} + \tilde{y}_{xxx}$ into the vector form (6.29), we obtain the equation

$$\tilde{y}_t + \frac{1}{6}B\tilde{y}_{xxx} + A(\bar{u},\bar{v})\tilde{y}_x = 0, \tag{6.31}$$

where we assume that $\bar{u}$ the constant solution and ignore higher order terms of $\tilde{y}$. With the aid of the decomposition of the matrix A with eigenvalues $\lambda_{1,2} = \bar{u} \pm \sqrt{v+1}$ and assuming $\lambda_1 = \lambda_2 = a$, we obtain

$$\begin{aligned} \tilde{u}_t + \frac{1}{6}\tilde{v}_{xxx} + a\tilde{u}_x &= 0 \\ \tilde{v}_t + \frac{1}{6}\tilde{u}_{xxx} + a\tilde{v}_x &= 0, \end{aligned} \tag{6.32}$$

which is the linearized version of (6.28) around the constant solution. The dispersion relations for the linearized equation (6.32) are

$$\begin{aligned} \omega_1 &= \frac{1}{6}k^3\frac{\tilde{v}}{\tilde{u}} - ak \\ \omega_2 &= \frac{1}{6}k^3\frac{\tilde{u}}{\tilde{v}} - ak, \end{aligned} \tag{6.33}$$

where the term $\tilde{v}/\tilde{u}$ is introduced as constant and it appears as a multiplier and a divisor for the dispersion relations in (6.33) [56].

In order to prove the dispersive property of the KdV-KdV equation, the phase velocities can be obtained as

$$\frac{\omega_1}{k} = \frac{k^2}{6}\frac{\tilde{v}}{\tilde{u}} - a, \quad \frac{\omega_2}{k} = \frac{k^2}{6}\frac{\tilde{u}}{\tilde{v}} - a.$$

Since the phase velocities with resect to the variables u and v are quadratic functions of the wave number k, they are both dispersive.

Contrary to the Ito's system whose dispersion relations for $\tilde{u}$ and $\tilde{v}$ were separated, in the KdV-KdV system the relations are related to each other by a constant term.

The continuous group velocities of the wave solutions u and v are computed by taking the first derivative of the equations in (6.33) with respect to k and obtained

$$\frac{d\omega_1}{dk} = \frac{1}{2}k^2\frac{\tilde{v}}{\tilde{u}} - a, \quad \frac{d\omega_2}{dk} = \frac{1}{2}k^2\frac{\tilde{u}}{\tilde{v}} - a, \tag{6.34}$$

where $\bar{\omega} = \omega\Delta t$ and $\bar{k} = k\Delta x$

6.1.2.3 Symmetric KdV-KdV System

The symmetric version of the KdV-KdV system (4.41) can be rewritten as follows

$$\begin{aligned} u_t + \frac{1}{6}v_{xxx} + \frac{3}{2}uu_x + \left(1 + \frac{1}{2}v\right)v_x = 0, \\ v_t + \frac{1}{6}u_{xxx} + (1 + \frac{1}{2}v)u_x + \frac{1}{2}uv_x = 0. \end{aligned} \tag{6.35}$$

As in the previous sections on coupled equations, to linearize (6.35), it has to be written in terms of vector $y = (u, v)^T$ such that

$$y_t + \frac{1}{6}By_{xxx} + A(u, v)y_x = 0, \tag{6.36}$$

where the 2×2 square matrix B is same as (6.30) and

$$A(u, v) = \begin{pmatrix} \frac{3}{2}u & \frac{1}{2}v + 1 \\ \frac{1}{2}v + 1 & \frac{1}{2}u \end{pmatrix}.$$

We linearize (6.36) around a constant solution $\bar{y} = (\bar{u}, \bar{v})^T$ with a small perturbation $\tilde{y} = (\tilde{u}, \tilde{v})^T$, where $|\tilde{u}|, |\tilde{v}| \ll 1$. When the solution y and its derivatives such that

$$y_t = \bar{y}_t + \tilde{y}_t, \quad y_x = \bar{y}_x + \tilde{y}_x, \quad y_{xxx} = \bar{y}_{xxx} + \tilde{y}_{xxx}$$

are inserted into (6.36) and simplified as in the previous sections, then we obtain

$$\tilde{y}_t + \frac{1}{6}B\tilde{y}_{xxx} + A(\bar{u}, \bar{v})\tilde{y}_x = 0. \tag{6.37}$$

As in the previous cases of coupled KdV equations, we take the equation (6.37) to apply the spectral decomposition to the matrix $A(\bar{u}, \bar{v})$ to write it as a diagonal matrix and hence to write in the linearized form. We can find the eigenvalues of the matrix A as

$$\lambda_{1,2} = \bar{u} \pm \sqrt{\bar{u}^2 - 4\bar{v}^2 - 4\bar{v} - 4}$$

and write it as $A = VDV^{-1}$, where the columns of the matrix V represent the eigenvectors of A. Once we multiply the equation (6.37) with V^{-1} from left and choose the eigenvalues to

be equal to each other and a constant a as $\lambda_1 = \lambda_2 = a$, we can get the following linearized equations

$$\begin{aligned} \tilde{u}_t + \frac{1}{6}\tilde{v}_{xxx} + a\tilde{u}_x &= 0 \\ \tilde{v}_t + \frac{1}{6}\tilde{u}_{xxx} + a\tilde{v}_x &= 0, \end{aligned} \tag{6.38}$$

which is exactly the same as (6.32). Now, since the linearized equations are the same for the equations (6.32) and (6.38), continuous dispersion relations and hence group velocities, which were found before in (6.33) and (6.34) will be the same. Also, it can be concluded that the phase velocities are equal, so the symmetric KdV-KdV system is dispersive as well.

6.2 Numerical Dispersion Relations

This section deals with the numerical dispersion relations of the same equations whose linearized forms and the continuous dispersion relations with the group velocities are found in the previous section. The numerical dispersion relations are obtained using the discrete version of the Fourier mode (6.5) [60]:

$$\tilde{u}_j^n = \hat{u}e^{i(jk\Delta x + n\omega\Delta t)}, \quad i = \sqrt{-1}. \tag{6.39}$$

To simplify the calculations, we continue with the solution u instead of $\tilde{u}$ for the linearized equations and also introduce the notation of $\bar{k} = k\Delta x$ and $\bar{\omega} = \omega\Delta t$, then (6.39) is written as

$$u_j^n = \hat{u}e^{i(j\bar{k} + n\bar{\omega})}. \tag{6.40}$$

In order to compare the discrete dispersion relation with the continuous one, the relation in the form (6.1) is rewritten as $\bar{\omega} = \bar{\omega}(\bar{k})$. The plots for the dispersion relations and the group velocities are drawn as $\bar{k}$ vs. $\bar{\omega}$, that is, $k\Delta x$ vs. $\omega\Delta t$ in the range $-\pi \leq k\Delta x, \omega\Delta t \leq \pi$, since the solutions are periodic in the intervals of length 2π. The periodicity of the solutions can be explained as follows:

The semi-discrete Fourier transform of (6.2) can be written as

$$\tilde{u}(x,t) = \Sigma_{j=-\infty}^{\infty} u_j(t) e^{-ikj\Delta x} e^{i\omega(k)t}\, \Delta x, \tag{6.41}$$

where $x_j = j\Delta x$.

Since the Euler's formula $e^{iy} = \cos y + i \sin y$ satisfies $e^{-i(2\pi m j)} = 1$, for any integer m, (6.41) can be written as

$$\tilde{u}(x,t) = \Sigma_{j=-\infty}^{\infty} u_j(t)\, e^{-ikj\Delta x}\, e^{i\omega(k)t}\, \Delta x = \Sigma_{j=-\infty}^{\infty} u_j(t)\, e^{-i(k+2\pi m/\Delta x)j\Delta x\; i\omega(k)t}\, \Delta x$$

and this tells us that any wave number k is indistinguishable from all other wave numbers $k + 2\pi m/\Delta x$, where $m \in \mathbb{Z}$. This is called aliasing. Hence, that proves $\bar{k}$, which is $k\Delta x$ is 2π periodic. The same can be done for semi-discretization in time for $\omega\Delta t$ to show that $\omega\Delta t$ is also 2π periodic.

The dispersion relations in this section are given for the first formulation of the bi-Hamiltonian systems, since both of the discretizations end up with the same result after applying the AVF method. Since there is only one pair to be considered, for simplicity we drop the sub numbers of the Hamiltonian functional and the operator, that is, $\mathcal{J}_1$ and $\mathcal{H}_2$ will be mentioned as $\mathcal{J}$ and $\mathcal{H}$, respectively.

6.2.1 KdV Equation

We consider, the linearized KdV equation (6.14) with the revised Hamiltonian operator and the Hamiltonian functional with respect to the first formulation

$$\mathcal{J} = D, \qquad \mathcal{H} = \int \left[\left(\frac{\alpha_1}{2} + \frac{\rho}{2}\right)u^2 - \frac{\nu}{2}u_x^2\right]dx. \tag{6.42}$$

Semi-discrete form of (6.42) is written as

$$\bar{J} = \frac{1}{2\Delta x}A, \quad \bar{H} = \sum_{j=1}^{N}\left[\left(\frac{\alpha_1}{2} + \frac{\rho}{2}\right)u_j^2 - \frac{\nu}{2\Delta x^2}(u_{j+1} - u_j)^2\right], \tag{6.43}$$

where A is the same matrix as (4.3).

Taking the gradient of $\bar{H}$ gives

$$\nabla\bar{H}(u_j) = (\alpha_1 + \rho)u_j + \frac{\nu}{\Delta x^2}(u_{j+1} - 2u_j + u_{j-1}) \quad \text{for} \quad j = 1, \ldots, N. \tag{6.44}$$

Then we apply the AVF method to the linearized KdV equation (6.14) and obtain

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2\Delta x}A\left[\frac{\alpha_1}{2}(u^{n+1} + u^n) + \frac{\rho}{2}(u^{n+1} + u^n) + \frac{\nu}{2\Delta x^2}(\tilde{u}^{n+1} + \tilde{u}^n)\right]. \tag{6.45}$$

When multiplied with the matrix A in (4.3), the equation (6.45) can be rewritten as

$$\begin{aligned}
\frac{u_j^{n+1} - u_j^n}{\Delta t} &+ \frac{\nu}{4\Delta x^3}(u_j^{n+1} - 2u_{j-1}^{n+1} + u_{j-2}^{n+1}) + \frac{\nu}{4\Delta x^3}(u_j^n - 2u_{j-1}^n + u_{j-2}^n) \\
&+ \frac{\alpha_1}{4\Delta x}(u_{j-1}^{n+1} + u_{j-1}^n) + \frac{\rho}{4\Delta x}(u_{j-1}^{n+1} + u_{j-1}^n) \\
&- \frac{\nu}{4\Delta x^3}(u_{j+2}^{n+1} - 2u_{j+1}^{n+1} + u_j^{n+1}) - \frac{\nu}{4\Delta x^3}(u_{j+2}^n - 2u_{j+1}^n + u_j^n) \\
&- \frac{\alpha_1}{4\Delta x}(u_{j+1}^{n+1} + u_{j+1}^n) - \frac{\rho}{4\Delta x}(u_{j+1}^{n+1} + u_{j+1}^n) = 0.
\end{aligned} \tag{6.46}$$

To obtain the numerical dispersion relation, we substitute (6.40) into (6.46) and simplify to get

$$\begin{aligned}(e^{i\omega\Delta t}-1) \quad &+ \quad \nu\frac{\Delta t}{\Delta x^3}(e^{-2i\bar{k}}-2e^{-i\bar{k}}+1)(e^{i\omega\Delta t}+1)-\nu\frac{\Delta t}{4\Delta x^3}(e^{2i\bar{k}}-2e^{i\bar{k}}+1)(e^{i\omega\Delta t}+1)\\ &+ \quad \alpha_1\frac{\Delta t}{4\Delta x}e^{-i\bar{k}}(e^{i\omega\Delta t}+1)-\alpha_1\frac{\Delta t}{4\Delta x}e^{i\bar{k}}(e^{i\omega\Delta t}+1)\\ &+ \quad \rho\frac{\Delta t}{4\Delta x}e^{-i\bar{k}}(e^{i\omega\Delta t}+1)-\rho\frac{\Delta t}{4\Delta x}e^{i\bar{k}}(e^{i\omega\Delta t}+1)=0.\end{aligned} \tag{6.47}$$

We consider two different approaches to obtain the discrete dispersion relation introduced in the joint work of Islas, Schober, Wlodarczyk [31] and of McLachlan's and Ascher's [2]. These two different approaches are applied to the Sine-Gordon equation in [60].

First approach: [31] Assuming that $\bar{k} \neq i\pi$, $w\Delta t \neq (2i+1)\pi$ for $i \in \mathbb{Z}$. Dividing both sides of the equation (6.47) by $(e^{i\omega\Delta t}+1)$, we obtain

$$\begin{aligned}\frac{e^{i\omega\Delta t}-1}{e^{i\omega\Delta t}+1} \quad &+ \quad \nu\frac{\Delta t}{4\Delta x^3}(e^{-2i\bar{k}}-2e^{-i\bar{k}}+1)-\nu\frac{\Delta t}{\Delta x^3}(e^{2i\bar{k}}-2e^{i\bar{k}}+1)\\ &+ \quad \alpha_1\frac{\Delta t}{\Delta x}(e^{-i\bar{k}}-e^{i\bar{k}})+\rho\frac{\Delta t}{\Delta x}(e^{-i\bar{k}}-e^{i\bar{k}})=0.\end{aligned} \tag{6.48}$$

Using the complex definition of the sine, cosine and tangent functions such that

$$\sin\theta=\frac{e^{i\theta}-e^{-i\theta}}{2}, \quad \cos\theta=\frac{e^{i\theta}+e^{-i\theta}}{2}, \quad \tan\theta=\frac{e^{2i\theta}-1}{e^{2i\theta}+1},$$

we arrive at

$$\tan(\frac{\omega\Delta t}{2})-\nu\frac{\Delta t}{\Delta x^3}[\sin\bar{k}(\cos\bar{k}-1)]-\left(\alpha_1\frac{\Delta t}{2\Delta x}+\rho\frac{\Delta t}{2\Delta x}\right)\sin\bar{k}=0. \tag{6.49}$$

When the continuous dispersion relation (6.15) and the numerical dispersion relation (6.49) are compared, it is seen that the AVF scheme does not preserve the form of the analytic dispersion relation (6.15).

To check the accuracy between the continuous dispersion relation (6.15) and the numerical dispersion relation (6.49), we take the limit of the numerical dispersion as $\Delta t, \Delta x \to 0$. For this, first we multiply (6.49) by $1/\Delta t$ and get

$$\frac{\tan(\frac{\omega\Delta t}{2})}{\Delta t}-\nu\left[\frac{\sin k\Delta x}{\Delta x}\left(\frac{\cos k\Delta x-1}{\Delta x^2}\right)\right]-\left(\frac{\alpha_1}{2}+\frac{\rho}{2}\right)\frac{\sin k\Delta x}{\Delta x}=0, \tag{6.50}$$

where the notations $\bar{k}$ is taken as $k\Delta x$. Now using the fact that

$$\lim_{\Delta t\to 0}\frac{\tan(\frac{\omega\Delta t}{2})}{\Delta t}=\frac{\omega}{2}, \quad \lim_{\Delta x\to 0}\frac{\sin k\Delta x}{\Delta x}=k \quad \text{and} \quad \lim_{\Delta x\to 0}\frac{\cos k\Delta x-1}{\Delta x^2}=-\frac{k^2}{2}$$

when we take the limit of (6.50) as $(\Delta t, \Delta x) \to (0, 0)$, we obtain

$$\omega + \nu k^3 - \alpha_1 k - \rho k = 0,$$

which is equivalent to (6.15). This shows us that the numerical dispersion relation tends to the continuous one for the ideal choice of Δt and Δx.

Moreover, we can rewrite (6.49)

$$\tan(\frac{\bar{\omega}}{2}) - \nu\frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k} - 1)] - \left(\alpha_1\frac{\lambda}{2} + \rho\frac{\lambda}{2}\right)\sin\bar{k} = 0, \tag{6.51}$$

where $\lambda = \frac{\Delta t}{\Delta x}$. This leads to the dispersion relation

$$\bar{\omega}(\bar{k}) = 2\arctan\left[\left(\nu\frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k} - 1)] + \left(\alpha_1\frac{\lambda}{2} + \rho\frac{\lambda}{2}\right)\sin\bar{k}\right)\right]. \tag{6.52}$$

The necessary condition to write the equation (6.51) as (6.52) is the invertibility of the tangent function. Tangent function is invertible on the interval $(-\pi/2, \pi/2)$, which corresponds to the condition $-\pi < \omega < \pi$ for ω. This is automatically satisfied since for the dispersion relation both ω and k are defined on the interval $[-\pi, \pi]$ as explained before at the beginning of this Chapter.

Now, we consider two terms of Maclaurin's series expansion for trigonometric terms in (6.49) and we get

$$\begin{aligned} \tan\left(\frac{\omega\Delta t}{2}\right) &= \frac{\omega\Delta t}{2} - \left(\frac{\omega\Delta t}{2}\right)^2 + O(\omega^3), \\ \sin\bar{k}\left(\cos\bar{k} - 1\right) &= -\frac{\bar{k}^3}{2} + \frac{\bar{k}^5}{8} + O\left(\bar{k}^7\right), \\ \sin\bar{k} &= \bar{k} - \frac{\bar{k}^3}{6} + O\left(\bar{k}^5\right). \end{aligned} \tag{6.53}$$

When we take the first term from each expansion the resulting relation is consistent with the continuous dispersion relation (6.15).

McLachlan's and Asher's approach: [2] In this approach all the terms are written with respect to cosine function as much as possible, instead of the tangent. Starting from the equation (6.47), we can rewrite it as

$$\frac{e^{i\omega\Delta t} - 1}{e^{i\omega\Delta t} + 1} - \nu\frac{\Delta t}{4\Delta x^3}\left(e^{i\bar{k}} - e^{-i\bar{k}}\right)(e^{-i\bar{k}} + e^{i\bar{k}} - 2) - \left(\alpha_1\frac{\Delta t}{4\Delta x} + \rho\frac{\Delta t}{4\Delta x}\right)\left(e^{i\bar{k}} - e^{-i\bar{k}}\right) = 0. \tag{6.54}$$

Using the fact that $\cos\theta = \frac{1}{2}\left(e^{i\theta} + e^{-i\theta}\right)$, (6.54) can be written as

$$\frac{\sin(\omega\Delta t) + \cos(\omega\Delta t) - 1}{\sin(\omega\Delta t) + \cos(\omega\Delta t) + 1} - \nu\frac{\Delta t}{\Delta x^3}[\sin\bar{k}(\cos\bar{k} - 1)] - \left(\alpha_1\frac{\lambda}{2} + \rho\frac{\lambda}{2}\right)\sin\bar{k} = 0. \tag{6.55}$$

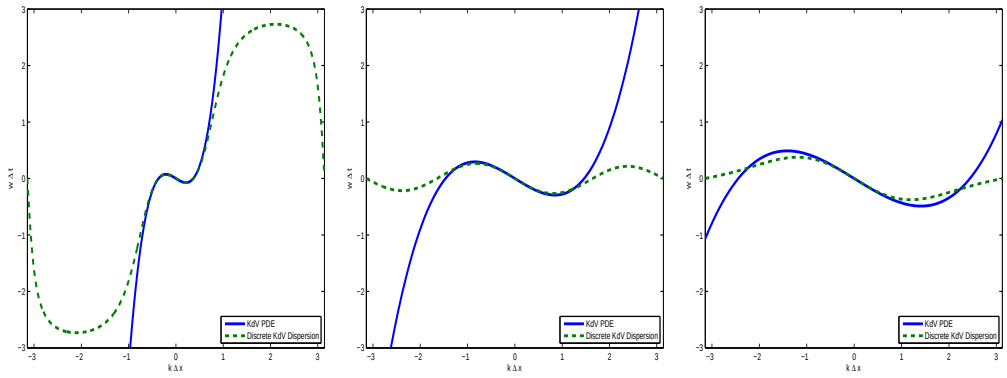
In the equation (6.55), when we consider the McLaurin's series expansion of the first term

$$\frac{\sin(\omega\Delta t)+\cos(\omega\Delta t)-1}{\sin(\omega\Delta t)+\cos(\omega\Delta t)+1}=\frac{\omega\Delta t}{2}-\left(\frac{\omega\Delta t}{2}\right)^2+O(\frac{\omega\Delta t}{3})$$

and using the identities in (6.53), we can see that first non-zero terms in the series expansion gives the continuous dispersion relation (6.15).

Similar to the result obtained for the sine-Gordon equation in [60], different approaches agree in the same result for the KdV equation in our work. Therefore, for the following equations, we will follow the first approach.

The continuous dispersion relation (6.15) and the numerical dispersion relation (6.49) with the coefficients $\alpha_1 = -2.6$, $\nu = -0.022^2$, $\rho = 0$ are displayed in Figure 6.1. To compare the dispersion curves with the results in [3] we have chose $\Delta x = 0.0005$, $\Delta x = 0.02$ and $\Delta x = 1/30$.



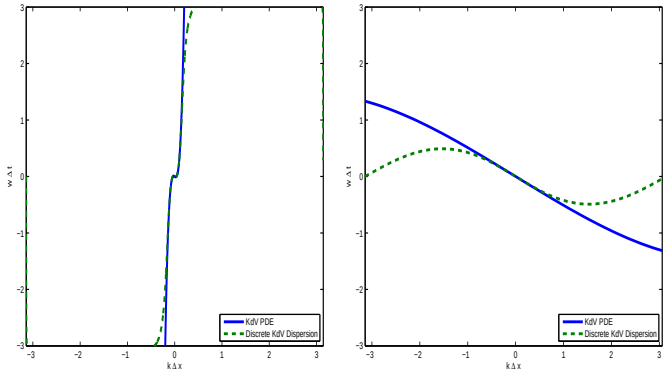
(a) $\Delta x = 0.0005$ (b) $\Delta x = 0.02$ (c) $\Delta x = 1/30$

Figure 6.1: Dispersion of the linearized KdV for $\lambda = 0.2$ and various values of Δx

The Figure 6.1 shows that the AVF method introduce numerical dispersion. It is seen that the dispersive properties of the AVF scheme is different for different Δx values. The dispersion curves in Figures 6.1(a)- 6.1(b) for the AVF method is below the analytical dispersion curve for $k > 0$. On the other hand, for $\Delta x = 1/30$, the dispersion curves for AVF make transitions from below to above the analytical curve at a value of the wave number $\bar{k}$ that depends on λ.

The Figure 6.1(a) shows that for the case that frequencies ω and the wave numbers k are both small, then the discrete dispersion is consistent with the theoretical dispersion. However, as they are getting larger in absolute value, then the discrete dispersion can not be catched by the theoretical one. The cases $\Delta x = 0.02$ and $\Delta x = 1/30$ with $\lambda = 0.2$ are displayed in

Figure 6.1(b) and 6.1(c), where the discrete scheme becomes closer to the exact linearized KdV for the larger frequency and wave number values in absolute. When we compare the dispersion graphs in Figure (6.1) with the curves in [3], we see that, the continuous and the numerical dispersion curves in Figure 6.1 show similar behavior as the dispersion curves in [3], where the latter results are obtained by midpoint rule. This is an expected result since the AVF method that we use is consistent with the midpoint rule. These conclusions give a rough estimate on the dispersion relation of the linearized KdV equation (6.14) such that the decrease in Δx by fixing other variables leads to the exact and discrete dispersions to be closer in the vertical axis. In a similar manner, when $\Delta x \sim 1$, the continuous and the numerical dispersion curves tend to each other in the horizontal axis as can be seen in Figure 6.2.



(a) $\Delta x = 0.0001$ (b) $\Delta x = 0.1$

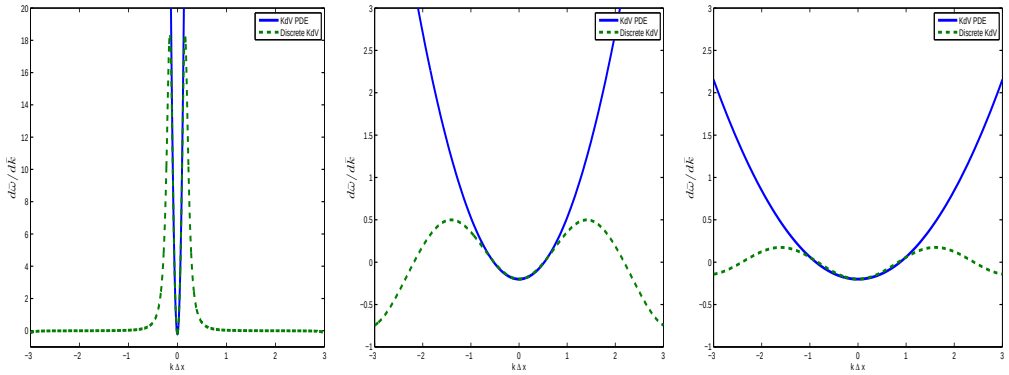
Figure 6.2: Dispersion of the linearized KdV for $\lambda = 0.2$, very small and big values of Δx

Taking the derivative of (6.52) with respect to k, where $k\Delta x$, we obtain the numerical group velocity

$$\frac{d\bar{\omega}}{d\bar{k}} = \lambda \frac{\frac{\nu}{\Delta x^2}\left(\cos^2\bar{k} - \sin^2\bar{k} - \cos\bar{k}\right) + (\frac{\alpha_1+\rho}{2})\left(\cos\bar{k}\right)}{1 + \left[\frac{\nu\Delta t}{\Delta x^3}\left[\sin\bar{k}\left(\cos\bar{k} - 1\right)\right] + (\frac{\alpha_1+\rho}{2})\frac{\Delta t}{\Delta x}\sin\bar{k}\right]^2}. \tag{6.56}$$

Figure 6.3 shows the graphs of the continuous group velocity (6.16) and the numerical group velocity (6.56) for different Δx values and $\lambda = 0.2$.

We can also compare the group velocities of the KdV equation that we have plotted in Figure 6.3 with the results obtained from the dispersion relations. The numerical dispersion relation is well preserved for different values of Δx when $\bar{k}$ is in the interval $(-1, 1)$. The slope of the dispersion curves in Figure 6.1, which corresponds to the group velocity $\bar{\omega}'(\bar{k})$, gives consistent information with the one obtained from Figure 6.3. That is, for the analytical



(a) $\Delta x = 0.0005$ (b) $\Delta x = 0.02$ (c) $\Delta x = 1/30$

Figure 6.3: Group velocity of the exact and discrete linearized KdV for $\lambda = 0.2$ and various values of Δx

dispersion, the curves are increasing on the interval $\bar{k} \in (-\pi, -0.8016) \cup (0.8384, \pi)$ and decreasing on the interval $\bar{k} \in (-0.8016, 0.8384)$ for $\Delta x = 0.0005$, or $\Delta x = 0.02$, or $\Delta x = 1/30$. When the continuous group velocity is investigated, we have seen that the sign of the group velocity is almost preserved, where $\bar{\omega}'(\bar{k}) > 0$ on the interval $\bar{k} \in (-\pi, -0.5416) \cup (0.5384, \pi)$ and $\bar{\omega}'(\bar{k}) < 0$ on the interval $\bar{k} \in (-0.5416, 0.5384)$. The continuous and the numerical group velocities in Figure 6.3 move close to each other up to some wave number, but then the numerical group velocity differ from the continuous one.

The group velocity curves in Figure 6.3 shows that the sign of the group velocity is not preserved by the AVF method.

6.2.2 mKdV Equation

The linearized mKdV (6.19) can be written as an infinite dimensional Hamiltonian system with

$$\mathcal{J} = D, \qquad \mathcal{H} = \int -\frac{1}{2}(au^2 - \nu u_x^2)\, dx, \tag{6.57}$$

where $a = \alpha \bar{u}^2$. Discretizing the Hamiltonian functional $\mathcal{H}$

$$\bar{H} = \sum_{j=1}^{N} -\frac{1}{2}\left[au_j^2 - \frac{\nu}{\Delta x^2}(u_{j+1} - u_j)^2\right]\Delta x,$$

we get the gradient of the Hamiltonian

$$\nabla \bar{H}(u_j) = au_j + \frac{\nu}{\Delta x^2}(u_{j+1} - 2u_j + u_{j-1}) \quad \text{for} \quad j = 1, \ldots, N. \tag{6.58}$$

Applying the average vector field method results in the following dispersion relation for the linearized mKdV equation (6.19), we get

$$\tan(\frac{\bar{\omega}}{2}) + a\frac{\lambda}{2}\sin\bar{k} + \nu\frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k}-1)] = 0, \tag{6.59}$$

which can be rewritten as

$$\bar{\omega}(\bar{k}) = 2\arctan\left(-a\frac{\lambda}{2}\sin\bar{k} - \nu\frac{\lambda}{\Delta x^2}\left[\sin\bar{k}(\cos\bar{k}-1)\right]\right), \tag{6.60}$$

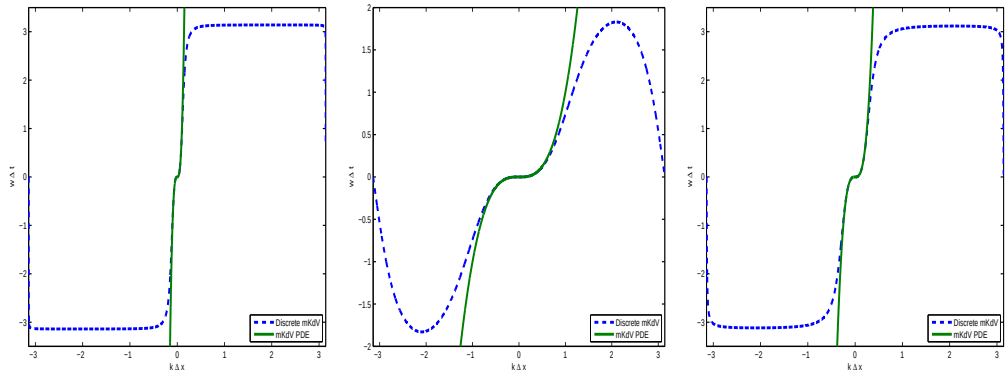
where $-\pi < \omega < \pi$.

Then one can find the discrete group velocity by taking the derivative of (6.60) with respect to k

$$\frac{d\bar{\omega}}{d\bar{k}} = \lambda\frac{\frac{\nu}{\Delta x^2}\left(\cos^2\bar{k} - \sin^2\bar{k} - \cos\bar{k}\right) - \frac{a}{2}\left(\cos\bar{k}\right)}{1 + \left[\frac{\nu\Delta t}{\Delta x^3}\left[\sin\bar{k}\left(\cos\bar{k}-1\right)\right] + \frac{a}{2}\frac{\Delta t}{\Delta x}\sin\bar{k}\right]^2}. \tag{6.61}$$

For the following dispersion relation and group velocity plots from now on, we will use various values for the mesh ratio λ with a constant time step $\Delta t = 0.001$.

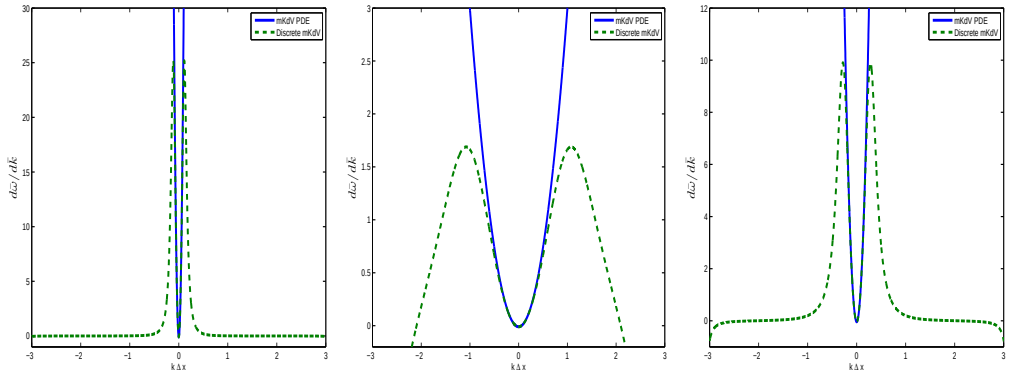
The difference between the exact and the approximate dispersion relations and the group velocities for the mKdV equation can be found in Figure 6.4 and 6.5,respectively, for $a = 1$ and $\nu = 1$.



(a) $\lambda = 0.1$ (b) $\lambda = 0.01$ (c) $\lambda = 0.04$

Figure 6.4: Dispersion of the linearized mKdV equation for $\Delta t = 0.001$, $a = 1$ and various values of λ.

When the discrete and the continuous cases are compared, according to Figure 6.4 the results that we obtained are similar to the KdV equation. That is, the curves move near to each other for small values of k, which corresponds to a long wave with a high frequency ω. However, for the large wave numbers the curves move away from each other as seen on Figure 6.4.



(a) $\lambda = 0.1$ (b) $\lambda = 0.01$ (c) $\lambda = 0.04$

Figure 6.5: Group velocities of the equation (6.19) for $\Delta t = 0.001$, $a = 1$ and various values of λ.

Moreover, as in the case of the KdV equation, the sign of the group velocity is not preserved exactly by the AVF method.

6.2.3 Ito's System

For the linearized Ito's system (6.25), we have to find the Hamiltonian functional and the operator regarding the new system. The corresponding pair of the Ito's system for the first Hamiltonian formulation becomes

$$\mathcal{J} = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}, \quad \mathcal{H} = \int \left(-\frac{u_x^2}{2} + \frac{a}{2}(u^2 + v^2) \right) dx, \tag{6.62}$$

where the constant a is chosen such that both of the eigenvalues (6.24) are equal to each other and also equal to a.

We apply the energy preserving method to the linearized Ito's system (6.25) with the Hamiltonian and the Hamiltonian operator in (6.62) by using the semi-discrete Hamiltonian functional is

$$\bar{H} = \sum_{j=1}^{N} \left(-\frac{1}{2\Delta x^2}(u_{j+1} - u_j)^2 - \frac{a}{2}(u_j^2 + v_j^2) \right) \Delta x$$

and its gradient

$$\nabla \bar{H}(u, v) = \begin{pmatrix} \frac{\partial \bar{H}}{\partial u} \\ \frac{\partial \bar{H}}{\partial v} \end{pmatrix},$$

where

$$\frac{\partial \bar{H}}{\partial u} = \begin{pmatrix} \frac{1}{\Delta x^2}(u_2 - 2u_1 + u_N) + au_1 \\ \vdots \\ \frac{1}{\Delta x^2}(u_{j+1} - 2u_j + u_{j-1}) + au_j \\ \vdots \\ \frac{1}{\Delta x^2}(u_1 - 2u_N + u_{N-1}) + au_N \end{pmatrix} \quad \text{and} \quad \frac{\partial \bar{H}}{\partial v} = \begin{pmatrix} av_1 \\ \vdots \\ av_j \\ \vdots \\ av_N \end{pmatrix}$$

for $j = 1, \ldots, N$. For the discretization of $\mathcal{J}$ in (6.62), we have used the matrix (4.35). Now, we can apply the AVF method in the vector form and when we make all computations using the first approach as in section (6.2.1), we can find the following dispersion relations

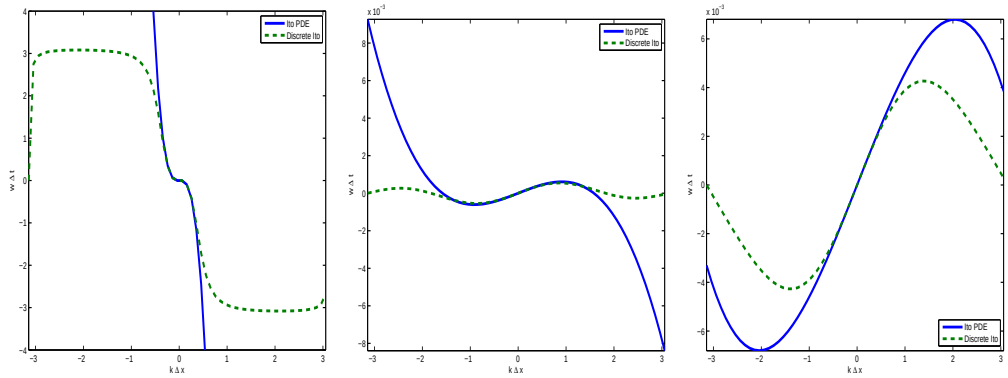
$$\begin{aligned} &\tan\left(\frac{\bar{\omega}_1}{2}\right) - \frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k} - 1)] - a\frac{\lambda}{2}\sin\bar{k} = 0, \\ &\tan\left(\frac{\bar{\omega}_2}{2}\right) - a\frac{\lambda}{2}\sin\bar{k} = 0, \end{aligned} \tag{6.63}$$

for u and v, respectively. These dispersion equations are equivalent to

$$\begin{aligned} \bar{\omega}_1 &= 2\arctan\left(\frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k} - 1)] + a\frac{\lambda}{2}\sin\bar{k}\right), \\ \bar{\omega}_2 &= 2\arctan\left(a\frac{\lambda}{2}\sin\bar{k}\right), \end{aligned} \tag{6.64}$$

where $-\pi < \omega_1, \omega_2 < \pi$.

One can easily show that the pair of equations (6.64) turn to (6.26) by expanding the McLaurin's series up to two terms.



(a) $a = 0.1$ and $\lambda = 0.4$ (b) $a = 0.1$ and $\lambda = 0.01$ (c) $a = 0.5$ and $\lambda = 0.01$

Figure 6.6: Dispersion curves for the solution u of the linearized Ito's system for $\Delta t = 0.05$ and various values of a and λ.

The curves corresponding to the continuous dispersion relation (6.26) and the discrete dispersion relations (6.64) for wave solution u can be found in Figure 6.6 for various values a and λ for $\Delta t = 0.05$.

Several observations can be made considering the Figure 6.6. The first is that the numerical dispersion introduced by the AVF method. Secondly, the dispersive properties of the AVF method are different. From the Figure 6.6, we see that numerical dispersion curves are above the analytical dispersion curve for $a = 0.1$, $\lambda = 0.4$ and $a = 0.1$, $\lambda = 0.01$, however an opposite situation is observed for $a = 0.5$, $\lambda = 0.01$.

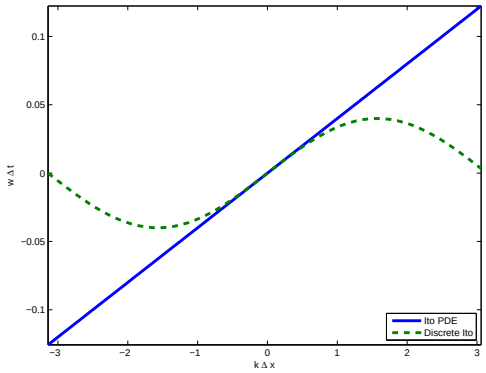


Figure 6.7: Travel of the wave solution v of the linearized Ito's system for $\Delta t = 0.05$, $a = 0.1$ and $\lambda = 0.4$

Since the wave solution v is not dispersive, in other words since the wave modes are traveling with a constant speed, the behavior is same for different values of a and λ. Therefore, the travel is shown by the single Figure 6.7. From the figure we see that the AVF method introduces the numerical dispersion, since the exact dispersion relation for v is linear and numeric dispersion relation for v is nonlinear.

The discrete group velocities then can be found by taking the derivative of (6.64) as

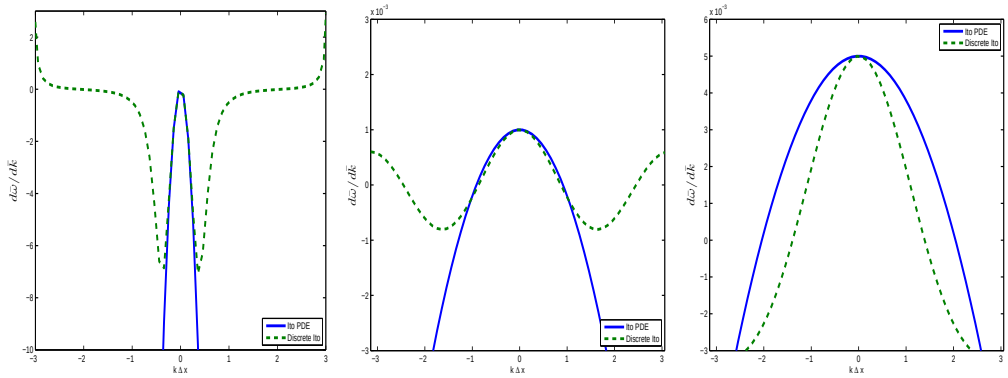
$$\begin{aligned} \frac{d\bar{\omega}_1}{d\bar{k}} &= \lambda \frac{\frac{1}{\Delta x^2}\left(\cos^2\bar{k} - \sin^2\bar{k} - \cos\bar{k}\right) - \frac{a}{2}\left(\cos\bar{k}\right)}{1 + \left[\frac{\Delta t}{\Delta x^3}\left[\sin\bar{k}\left(\cos\bar{k} - 1\right)\right] + \frac{a}{2}\frac{\Delta t}{\Delta x}\sin\bar{k}\right]^2} \\ \frac{d\bar{\omega}_2}{d\bar{k}} &= \lambda \frac{\frac{a}{2}\cos\bar{k}}{1 + \left(\frac{a}{2}\frac{\Delta t}{\Delta x}\sin\bar{k}\right)^2}. \end{aligned} \tag{6.65}$$

and compared with the continuous group velocities (6.27) in Figure 6.8, which are

$$\frac{d\bar{\omega}_1}{d\bar{k}} = -3\frac{\lambda}{\Delta x^2}\bar{k}^2 + a\lambda, \quad \frac{d\bar{\omega}_2}{d\bar{k}} = a\lambda$$

to understand the behaviors of the waves.

Figure 6.8 shows that the group velocity curves of the AVF method are very close to the analytical one for $a = 0.1$. Although the analytical group velocity curves are monotonically



(a) $a = 0.1$ and $\lambda = 0.4$ (b) $a = 0.1$ and $\lambda = 0.01$ (c) $a = 0.5$ and $\lambda = 0.01$

Figure 6.8: Group velocities of the solution u of the linearized Ito's system for $\Delta t = 0.05$ and various values of a and λ.

decreasing for $k > 0$, the group velocity curve for the AVF method is not monotone. Moreover, the sign of the group velocity is not preserved by the AVF method.

6.2.4 KdV-KdV and Symmetric KdV-KdV System

In this section, the dispersion relations and the group velocities of the linearized KdV-KdV (6.32) and the symmetric KdV-KdV (6.38) systems are examined together, since they have the same linearized coupled equations and that leads to same dispersion relations, hence leads to same group velocities.

We consider the equations (6.32) and (6.38), their infinite Hamiltonian formulations have to be revised as in the following way.

The linearized equation (6.32) can be reformulated as an infinite Hamiltonian system by using

$$\mathcal{J} = \begin{pmatrix} \frac{D}{2} & 0 \\ 0 & \frac{D}{2} \end{pmatrix}, \quad \mathcal{H} = \int \left(\frac{1}{6} \left(u_x^2 + v_x^2 \right) - 2auv \right) dx, \tag{6.66}$$

where a is constant. The spatial discretization of the Hamiltonian operator $\mathcal{J}$ is obvious (see (4.35)) and the Hamiltonian functional takes the form

$$\bar{H} = \sum_{j=1}^{N} \left[\frac{1}{6\Delta x^2} \left((u_{j+1} - u_j)^2 + (v_{j+1} - v_j)^2 \right) - 2au_j + v_j \right] \Delta x.$$

Then the gradient of $\bar{H}$ can be computed as

$$\nabla \bar{H}(u,v) = \begin{pmatrix} \frac{\partial \bar{H}}{\partial u} \\ \frac{\partial \bar{H}}{\partial v} \end{pmatrix} = \begin{pmatrix} -\frac{1}{3\Delta x^2}\left(u_2 - 2u_1 + u_N\right) - 2av_1 \\ \vdots \\ -\frac{1}{3\Delta x^2}\left(u_{j+1} - 2u_j + u_{j-1}\right) - 2av_j \\ \vdots \\ -\frac{1}{3\Delta x^2}\left(u_1 - 2u_N + u_{N-1}\right) - 2av_N \\ -\frac{1}{3\Delta x^2}\left(v_2 - 2v_1 + v_{N-1}\right) - 2au_N \\ \vdots \\ -\frac{1}{3\Delta x^2}\left(v_{j+1} - 2v_j + v_{j-1}\right) - 2au_j \\ \vdots \\ -\frac{1}{3\Delta x^2}\left(v_1 - 2v_N + v_{N-1}\right) - 2au_N \end{pmatrix},$$

where $j = 1, \ldots, N$.

Before we move on to the discrete dispersion relation, let us also write the new Hamiltonian formulation of the linearized symmetric KdV-KdV system (6.38). The corresponding Hamiltonian operator and the functional are

$$\mathcal{J} = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}, \quad \mathcal{H} = \int \left(-\frac{uv_{xx}}{6} - \frac{a}{2}\left(u^2 + v^2\right)\right) dx. \tag{6.67}$$

Then the semi-discrete Hamiltonian and its gradient are obtained as

$$\bar{H} = \sum_{j=1}^{N} \left[\frac{u_j\left(v_{j+1} - 2v_j + v_{j-1}\right)}{6\Delta x^2} - \frac{a}{2}\left(u_j^2 + v_j^2\right)\right]\Delta x$$

$$\nabla \bar{H}(u,v) = \begin{pmatrix} \frac{\partial \bar{H}}{\partial u} \\ \frac{\partial \bar{H}}{\partial v} \end{pmatrix} = \begin{pmatrix} -\frac{v_2 - 2v_1 + v_N}{6\Delta x^2} - au_1 \\ \vdots \\ -\frac{v_{j+1} - 2v_j + v_{j-1}}{6\Delta x^2} - au_j \\ \vdots \\ -\frac{v_1 - 2v_N + v_{N-1}}{6\Delta x^2} - au_N \\ -\frac{u_2 - 2u_1 + u_N}{6\Delta x^2} - av_1 \\ \vdots \\ -\frac{u_{j+1} - 2u_j + u_{j-1}}{6\Delta x^2} - av_j \\ \vdots \\ -\frac{u_1 - 2u_N + u_{N-1}}{6\Delta x^2} - av_N \end{pmatrix},$$

where $j = 1, \ldots, N$.

When we apply the AVF method to both Hamiltonian pairs (6.66) and (6.67), we get the following common dispersion relations

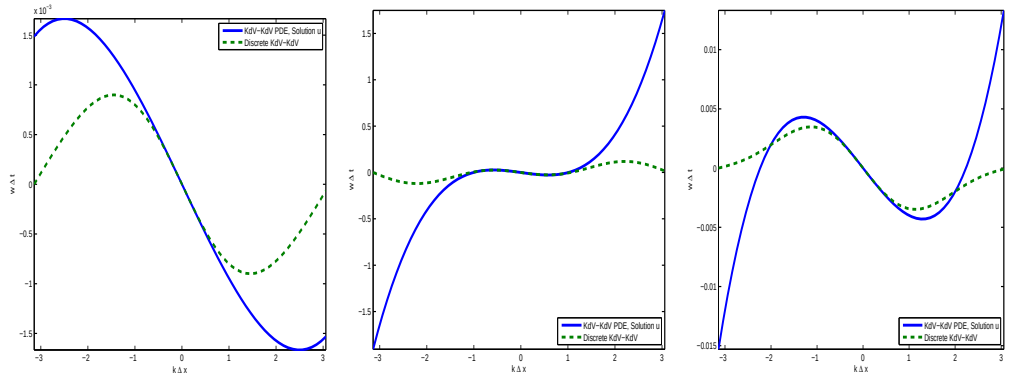
$$\begin{aligned} \tan\left(\frac{\bar{\omega}_1}{2}\right) + \frac{\lambda}{6\Delta x^2}[\sin\bar{k}(\cos\bar{k}-1)]\frac{\tilde{v}}{\tilde{u}} + a\frac{\lambda}{2}\sin\bar{k} = 0, \\ \tan\left(\frac{\bar{\omega}_2}{2}\right) + \frac{\lambda}{6\Delta x^2}[\sin\bar{k}(\cos\bar{k}-1)]\frac{\tilde{u}}{\tilde{v}} + a\frac{\lambda}{2}\sin\bar{k} = 0, \end{aligned} \tag{6.68}$$

which are equivalent to

$$\begin{aligned} \bar{\omega}_1 &= 2\arctan\left(-\frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k}-1)]\frac{\tilde{v}}{\tilde{u}} - a\frac{\lambda}{2}\sin\bar{k}\right), \\ \bar{\omega}_2 &= 2\arctan\left(-\frac{\lambda}{\Delta x^2}[\sin\bar{k}(\cos\bar{k}-1)]\frac{\tilde{u}}{\tilde{v}} - a\frac{\lambda}{2}\sin\bar{k}\right). \end{aligned} \tag{6.69}$$

The numerical dispersion relation (6.68) for the AVF method shows that the form of the analytical dispersion relation (6.33) is not preserved.

The comparison between the continuous (6.33) and the discrete (6.69) dispersion equations can be done by Figures 6.9 and 6.10 with respect to u and v for different choices of values for a, λ and $\frac{\tilde{v}}{\tilde{u}}$.

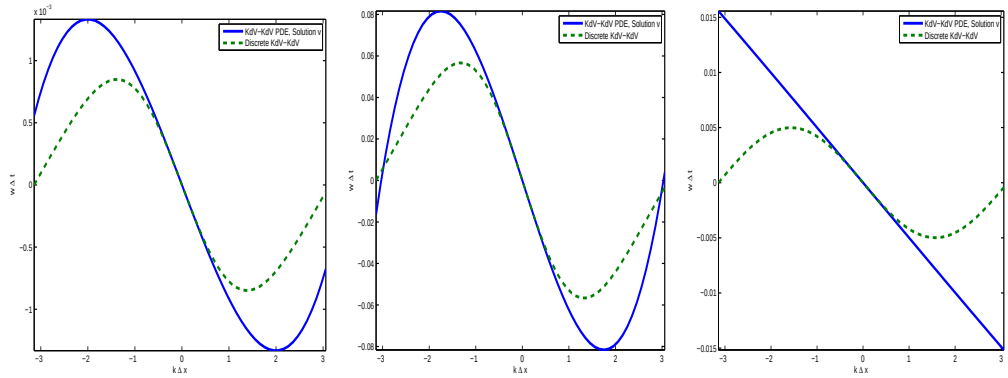


(a) $a = 0.1$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 0.8$ (b) $a = 1$, $\lambda = 0.07$ and $\frac{\tilde{v}}{\tilde{u}} = 3$ (c) $a = 0.5$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 15$

Figure 6.9: Dispersion curves for the solution u of the linearized KdV-KdV and symmetric KdV-KdV systems for $\Delta t = 0.05$ and various values of a, λ and $\frac{\tilde{v}}{\tilde{u}}$.

Then the group velocity of the linearized KdV-KdV systems can be obtained from the first derivative of the dispersion relations (6.69) as

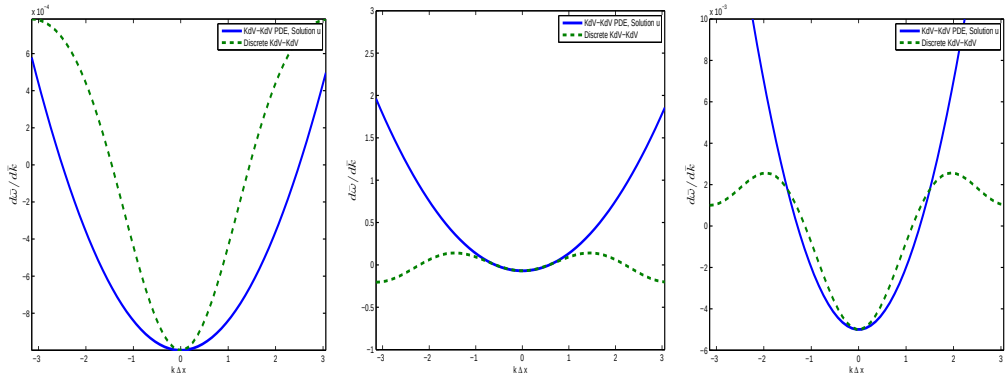
$$\begin{aligned} \frac{d\bar{\omega}_1}{d\bar{k}} &= \lambda\frac{\frac{1}{6\Delta x^2}\left(\cos^2\bar{k} - \sin^2\bar{k} - \cos\bar{k}\right)\frac{\tilde{v}}{\tilde{u}} - \frac{a}{2}\left(\cos\bar{k}\right)}{1 + \left[\frac{\Delta t}{6\Delta x^3}\frac{\tilde{v}}{\tilde{u}}\left[\sin\bar{k}\left(\cos\bar{k}-1\right)\right] + \frac{a}{2}\frac{\Delta t}{\Delta x}\sin\bar{k}\right]^2}, \\ \frac{d\bar{\omega}_2}{d\bar{k}} &= \lambda\frac{\frac{1}{6\Delta x^2}\left(\cos^2\bar{k} - \sin^2\bar{k} - \cos\bar{k}\right)\frac{\tilde{u}}{\tilde{v}} - \frac{a}{2}\left(\cos\bar{k}\right)}{1 + \left[\frac{\Delta t}{6\Delta x^3}\frac{\tilde{u}}{\tilde{v}}\left[\sin\bar{k}\left(\cos\bar{k}-1\right)\right] + \frac{a}{2}\frac{\Delta t}{\Delta x}\sin\bar{k}\right]^2}. \end{aligned} \tag{6.70}$$



(a) $a = 0.1$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 0.8$ (b) $a = 1$, $\lambda = 0.07$ and $\frac{\tilde{v}}{\tilde{u}} = 3$ (c) $a = 0.5$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 15$

Figure 6.10: Dispersion curves for the solution v of the linearized KdV-KdV and symmetric KdV-KdV systems for $\Delta t = 0.05$ and various values of a, λ and $\frac{\tilde{v}}{\tilde{u}}$.

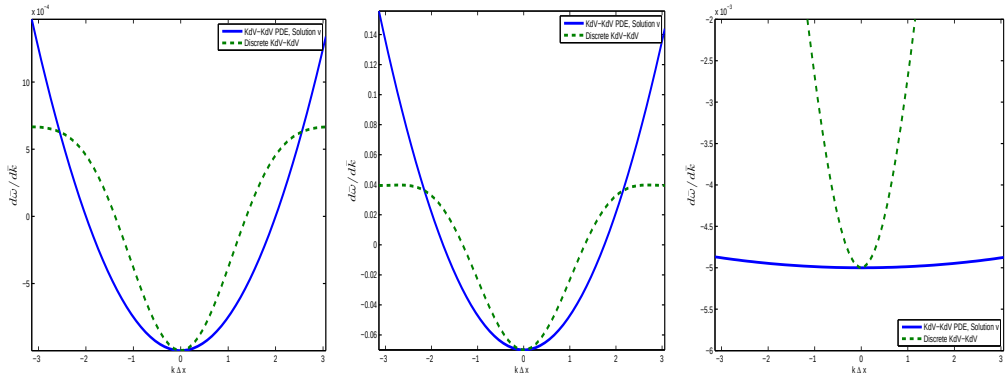
When the curves of the continuous (6.34) and the discrete (6.70) group velocities can be seen in Figures (6.11) and (6.12) for u and v, respectively.



(a) $a = 0.1$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 0.8$ (b) $a = 1$, $\lambda = 0.07$ and $\frac{\tilde{v}}{\tilde{u}} = 3$ (c) $a = 0.5$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 15$

Figure 6.11: Group velocities of the solution u of the linearized KdV-KdV and symmetric KdV-KdV systems for $\Delta t = 0.05$ and various values of a and λ.

As we have seen in the previous sections, the AVF method introduces numerical dispersion. In addition, the dispersive properties of the AVF method are distinct with respect to the different



(a) $a = 0.1$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 0.8$ (b) $a = 1$, $\lambda = 0.07$ and $\frac{\tilde{v}}{\tilde{u}} = 3$ (c) $a = 0.5$, $\lambda = 0.01$ and $\frac{\tilde{v}}{\tilde{u}} = 15$

Figure 6.12: Group velocities of the solution v of the linearized KdV-KdV and symmetric KdV-KdV systems for $\Delta t = 0.05$ and various values of a and λ.

initial conditions used to solve the equations.

CHAPTER 7

CONCLUSIONS

In this thesis, the energy preserving AVF method is applied the to KdV type Hamiltonian equations. The numerical results confirm the excellent long time preservation of the energy (Hamiltonian) and the other invariants of the underlying equations. The numerically obtained soliton solutions show a very similar behavior with those in the literature obtained by other methods.

With full discretization of the nonlinear equations, AVF method results in the implicit equations and to solve these equations Newton's method is used within machine accuracy. In this iterative manner, for each time step the result is obtained after at most 3 iterations and this leads to an increase in the cost of computation substantially. An alternative to reduce the computational cost would be using linearly implicit energy preserving methods as introduced in [20].

Once we obtained the results, there exist small oscillations around some of the solutions. The reason of this comes from the third order derivative in the equations and leads to dispersion. Therefore, a thorough dispersion analysis of the AVF method is carried out. When the exact and the numerical dispersion relations are compared, it is seen that for small wave numbers the dispersion curves show close behavior. However, as the wave number is getting larger in absolute value the numerical dispersion curves fail to catch the exact dispersion relation for all equations. On the other side, for large wave numbers the continuous (exact) group velocity does not match to the numerical one. Therefore, we concluded that there exists no diffeomorphism for the discrete dispersion relations, so that the sign of the group velocity is not preserved. This shows the weakness of the AVF method compared with the other structure preserving methods such as symplectic and multsymplectic integrators.

REFERENCES

[1] U. M. Ascher. *Numerical methods for evolutionary differential equations*. Society for Industrial and Applied Mathematics (SIAM), 2008.

[2] U. M. Ascher and R. I. McLachlan. Multisymplectic box schemes and the Korteweg-de Vries equation. *Appl. Numer. Math.*, 48:255–269, 2004.

[3] U. M. Ascher and R. I. McLachlan. On symplectic and multisymplectic schemes for the KdV equation. *J. Sci. Comput.*, 25:83–104, 2005.

[4] A. Aubry and P. Chartier. Pseudo symplectic runge-kutta methods. *BIT*, 38:439–461, 1998.

[5] A. Aydın and B. Karasözen. Multisymplectic box schemes for the complex modified Korteweg-de Vries equation. *J. Math. Phys.*, 51:083511, 24, 2010.

[6] J. Benn. The structure of B- series. Master's thesis, Massey University, New Zealand, 2010.

[7] M. Blaszak. *Multi-Hamiltonian Theory of Dynamical Systems*. Springer, 1998.

[8] J. L. Bona, V. A. Dougalis, and D. E. Mitsotakis. Numerical solution of KdV-KdV systems of Boussinesq equations. I. The numerical scheme and generalized solitary waves. *Math. Comput. Simulation*, 74:214–228, 2007.

[9] J. L. Bona, V. A. Dougalis, and D. E. Mitsotakis. Numerical solution of Boussinesq systems of KdV-KdV type. II. Evolution of radiating solitary waves. *Nonlinearity*, 21:2825–2848, 2008.

[10] K. Brauer. The Korteweg-de Vries Equation: History, exact solutions, and graphical representation. http://www.usf.uni-osnabrueck.de/ kbrauer/solitons/KdV.pdf, 2000.

[11] E. Celledoni, V. Grimm, R. I. McLahlan, D. I. McLaren, D. R. J. O'Neale, B. Owren, and G. R. W. Quispel. Preserving energy resp. dissipation in numerical pdes, using the Average Vector Field method. Technical Report 7/2009, Norwegian University of Science and Technology Trondheim, Norway, 2009. Available at http://www.math.ntnu.no/preprint/numerics/2009/N7-2009.ps.

[12] E. Celledoni, R. I. McLachlan, D. I. McLaren, B. Owren, G. R. W. Quispel, and W. M. Wright. Energy-preserving Runge-Kutta methods. *M2AN Math. Model. Numer. Anal.*, 43:645–649, 2009.

[13] E. Celledoni, R. I. McLahlan, B. Owren, and G. R. W. Quispel. Energy-preserving integrators and the structure of B-series. Technical Report 5/2009, Norwegian University of Science and Technology Trondheim, Norway, 2009. Available at http://www.math.ntnu.no/preprint/numerics/2009/N5-2009.ps.

[14] S. H. Christiansen, H. Z. Munthe-Kaas, and B. Owren. Topics in structure-preserving discretization. *Acta Numerica*, 20:1–119, 2011.

[15] D. Cohen and E. Hairer. Linear energy-preserving integrators for poisson systems. *BIT Numerical Mathematics*, 51:91–101, 2011.

[16] R. Courant, K. Friedrichs, and H. Lewy. On the partial difference equations of mathematical physics. *IBM J.*, 11:215–234, 1967.

[17] M. Dahlby and B. Owren. A general framework for deriving integral preserving numerical methods for PDEs. Technical Report 8/2010, Norwegian University of Science and Technology Trondheim, Norway, 2010. Available at http://www.math.ntnu.no/preprint/numerics/2010/N8-2010.ps.

[18] P. G. Drazin and R. S. Johnson. *Solitons: an introduction*. Cambridge University Press, 1989.

[19] B.-F. Feng and G. W. Wei. A comparison of the spectral and the discrete singular convolution schemes for the KdV-type equations. *J. Comput. Appl. Math.*, 145:183–188, 2002.

[20] D. Furihata and T. Matsuo. *Discrete Variational Derivative Method: A Structure-Preserving Numerical Method for Partial Differential Equations*. Chapman and Hall, 2010.

[21] C. S. Gardner, J. M. Greene, M. D. Kruskal, and R. M. Miura. Method for solving korteweg-de vries equation. *Phys. Rev Lett.*, 19:1095–1097, 1967.

[22] Ü. Göktaş and W. Hereman. Symbolic computation of conserved densities for systems of nonlinear evolution equations. *J. Symbolic Comput.*, 11:1–31, 2008.

[23] O. Gonzalez. Time integration and discrete Hamiltonian systems. *J. Nonlinear Sci.*, 6:449–467, 1996.

[24] D. F. Griffiths and D. J. Higham. *Numerical Methods for Ordinary Differential Equations: Initial Value Problems*. Springer, 2010.

[25] R. Grimshaw. Korteweg-de vries equation. In Scott A., editor, *Encyclopedia of Nonlinear Science*. Routledge, Taylor and Francis Group, 2004.

[26] P. Guha. Geodesic flows, bi-hamiltonian structure and coupled KdV type systems. *J. Math. Anal. Appl.*, 310:45–56, 2005.

[27] E. Hairer. Energy-preserving variant of collocation methods. *J. Numer. Anal. Ind. Appl. Math.*, 5:73–84, 2010.

[28] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration–Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer, 2006.

[29] A. Harten, P.D. Lax, and B. van Leer. On upstream differencing and Godunov-type schemes for hyperbolic conservation laws. *SIAM Review*, 25:35–61, 1983.

[30] A. Iserles, R. I. McLachlan, and A. Zanna. Approximately preserving symmetries in the numerical integration of ordinary differential equations. *Eur. J. Appl. Math.*, 10:419–445, 1999.

[31] A. Islas, C.M. Schober, and T.H. Wlodarczyk. Geometric integrators for the sine-gordon equation. Available at http://www.math.ucf.edu/ cschober/TOMASZ.pdf, 2006.

[32] M. Ito. An extension of nonlinear evolution equations of the K-dV (mK-dV) type to higher orders. *J. Phys. Soc. Japan*, 49:771–778, 1980.

[33] B. Karasözen. Poisson integrators. *Math. Comput. Modelling*, 40:1225–1244, 2004.

[34] D. J. Korteweg and G. de Vries. On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves. *Phil. Mag.*, 39:422–443, 1895.

[35] B. Leimkuhler and S. Reich. *Simulating Hamiltonian Dynamics*. Cambridge Univesity Press, 2004.

[36] Q. P. Liu. Hamiltonian structures for Ito's equation. *Phys. Lett. A*, 277:31–34, 2000.

[37] F. Magri. A short introduction to Hamiltonian PDEs. *Mat. Contemp.*, 15:213–230, 1998.

[38] L. Maicun. Equatorial solitary waves of tropical atmospheric motion in shear flow. *Advances in Atmospheric Sciences*, 2:125–136, 1987.

[39] R. I. McLachlan. Spatial discretization of partial differential equations with integrals. *IMA J. Numer. Anal.*, 23:645–664, 2003.

[40] R. I. McLachlan and G. R. W. Quispel. Generating functions for dynamical systems with symmetries, integrals, and differential invariants. *Phys. D*, 112:298–309, 1998.

[41] R. I. McLachlan, G. R. W. Quispel, and N. Robidoux. Geometric integration using discrete gradients. *R. Soc. Lond. Philos. Trans. Ser. A Math. Phys. Eng. Sci.*, 357:1021–1045, 1999.

[42] R. I. McLachlan, G. R. W. Quispel, and G. S. Turner. Numerical integrators that preserve symmetries and reversing symmetries. *SIAM J. Numer. Anal.*, 35:586–599, 1998.

[43] R. M. Miura. Korteweg-de vries equation and generalizations. I: A remarkable explicit nonlinear transformation. *J. Math. Phys.*, 9:1202–1204, 1968.

[44] P. J. Morrison. Hamiltonian description of the ideal fluid. *Rev. Mod. Phys.*, 70:467–521, 1998.

[45] G. A. Nariboli. Nonlinear longitudinal dispersive waves in elastic rods. *J. Math. Phys. Sci.*, 4:64–73, 1969.

[46] P. Olver. *Applications of Lie Groups to Differential Equations*. Springer, second edition, 1995.

[47] P. J. Olver and P. Rosenau. Tri-Hamiltonian duality between solitons and solitary-wave solutions having compact support. *Phys. Rev. E (3)*, 53:1900–1906, 1996.

[48] G. R. W. Quispel and H. W. Capel. Solving ODEs numerically while preserving a first integral. *Phys. Lett. A*, 218:223–228, 1996.

[49] G. R. W. Quispel and D. I. McLaren. A new class of energy-preserving numerical integration methods. *J. Phys. A*, 41:045206, 7, 2008.

[50] S. J. Russell. Report on waves. *Rep. 14th Meeting of the British Assoc. for the Advancement of Science, John Murray, London*, pages 311–390 + 11 plates, 1844.

[51] J. M. Sanz-Serna and M. P. Calvo. *Numerical Hamiltonian Problems*. Chapman and Hall, 1994.

[52] C. M. Schober and T. H. Wlodarczyk. Dispersive properties of multisymplectic integrators. *J. Comput. Phys.*, 227:5090–5104, 2008.

[53] C. M. Schober and T. H. Wlodarczyk. Dispersion, group velocity, and multisymplectic discretizations. *Math. Comput. Simulation*, 80:741–751, 2009.

[54] Jie Shen. A new dual-Petrov-Galerkin method for third and higher odd-order differential equations: application to the KdV equation. *SIAM J. Numer. Anal.*, 41:1595–1619, 2003.

[55] J. W. Thomas. *Numerical Partial Differential Equations: Finite Difference Methods*. Springer, 1995.

[56] L. N. Trefethen. *Finite Diference and Spectral Methods for Ordinary and Partial Differential Equations*. Cornell University, 1996.

[57] P. S. P. Tse. *Geometric Numerical Integration: On the Numerical Preservation of Multiple Geometric Properties for Ordinary Differential Equations*. PhD thesis, La Trobe University, Australia, 2007.

[58] H. Washimi and Taniuti T. Propagation of ion-acoustic solitary waves of small amplitude. *Phys. Rev. Lett*, 17:996–998, 1966.

[59] G. B. Whitham. *Linear and Nonlinear Waves*. John Wiley and Sons, 1974.

[60] T. H. Wlodarczyk. *Stability and Preservation Properties of Multisymplectic Integrators*. PhD thesis, University of Central Florida, Orlando, 2007.

[61] Y. Xu and C.-W Shu. Local discontinuous Galerkin methods for the Kuramoto-Sivashinsky equations and the Ito-type coupled KdV equations. *Comput. Methods Appl. Mech. Engrg.*, 195:3430–3447, 2006.

[62] N. J. Zabusky and M. D. Kruskal. Interaction of solitons in a collisionless plasma and the recurrence of initial states. *Phys. Rev. Let.*, 15:240–243, 1965.

[63] V. E. Zakharov and L. D. Faddeev. Korteweg-de vries equation: a completely integrable hamiltonian system. *Functional Anal. Appl.*, 5:280–287, 1972.

[64] P. F. Zhao and M. Z. Qin. Multisymplectic geometry and multisymplectic Preissmann scheme for the KdV equation. *J. Phys. A*, 33:3613–3626, 2000.

[65] C. Zheng. Numerical simulation of a modified KdV equation on the whole real axis. *Numer. Math.*, 105:315–335, 2006.