NON-STANDARD DISCRETIZATIONS OF DIFFERENTIAL EQUATIONS

A THESIS SUBMITTED TO

THE UNIVERSITY OF KENT AT CANTERBURY

IN THE SUBJECT OF MATHEMATICS

FOR THE DEGREE

OF DOCTOR OF PHILOSOPHY BY RESEARCH

By

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December 2015

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Abstract

This thesis explores non-standard numerical integration methods for a range of non-linear systems of differential equations with a particular interest in looking for the preservation of various features when moving from the continuous system to a discrete setting. Firstly the exsiting non-standard schemes such as one discovered by Hirota and Kimura (and also Kahan) [21, 32] will be presented along with general rules for creating an effective numerical integration scheme devised by Mickens [40].

We then move on to the specific example of the Lotka-Volterra system and present a method for finding the most general forms of a non-standard scheme that is both symplectic and birational. The resulting three schemes found through this method have also been discovered through an alternative method by Roeger in [52].

Next we look at discretizing examples of 3-dimensional bi-Hamiltonian systems from a list given by Gümral and Nutku [18] using the Hirota-Kimura/Kahan method followed by the same method applied to the Hénon-Heiles case (ii) system. The Bäcklund transformation for the Hénon-Heiles is also considered.

Finally chapter 6 looks at systems with cubic vector fields and limit cycles with an aim to find the most general form of a non-standard scheme for two examples. First we look at a trimolecular system and then a Hamiltonian system that has a quartic potential.

Acknowledgments

I would like to thank my supervisor Professor Andy Hone for his amazing support throughout my research, his kindness and understanding and his patience. He has been generous with his time in helping me and offering me guidance and direction when I would have otherwise been lost.

I am very grateful to my department and in particular I am very grateful to Claire Carter for her guidance and understanding with the administration and organisation of various elements of my time as a postgraduate. I would also like to thank Dr Jing Ping Wang for her helpful comments and corrections as a temporary supervisor when Professor Hone was away. I would also like to acknowledge EPSRC for funding my research.

I am immensely grateful to my partner Jamie for his support looking after our sons and his encourgement to keep going. Thank-you also to my parents for always being so encouraging and supportive towards my education.

Contents

Chapter 1

Introduction

This thesis is concerned with non-standard numerical integration methods for non-linear systems of differential equations, with a particular focus on preserving features of the continuous system through the discretization process. We mainly consider continuous systems that are Hamiltonian in nature.

1.1 Motivation

As there are plenty of systems of differential equations that can only be solved numerically it is vital that effective discretization methods are devised, and the search for such schemes that also preserve the structural properties of the original system are fundamental to numerical analysis. One of the first suggestions of a non-standard (not the typical known numerical schemes) discretization method came in the form of unpublished lecture notes by Kahan in 1993 in which he presented a method for discretizing a set of differential equations in which all of the components of the vector field are quadratic. One of the systems that Kahan applied this scheme to was the Lotka-Volterra system, and he found that it peserved the strucural properties of the original continuous system. There was no accompanying explanation as to how the scheme was devised or why it worked so well.

A few years later Hirota and Kimura independently rediscovered this discretization method, but this time applied to mechanics, and more specifically to the Euler Top system [21]. This prompted further interest and as a result new integrable maps were found, for example [27]. Although this new 'unconventional' method had been sucessfully used many times to produce new maps, there was still a lot of mystery around the conditions for which a map that preserves a symplectic structure and one of more first integrals is produced. Recently there has been more progress made with Celledoni et al [7] showing that Kahan's method actually coincides with the Runge-Kutta method applied to quadratic vector fields. Celledoni et al also went on to propose that if the continous system is a Hamiltonian system with a constant Poisson structure and a cubic Hamiltonian then the corresponding map has a rational first integral and peserves a volume form. In this thesis this Kahan/Hirota/Kimura scheme will be applied to further examples of continous systems such as 3-dimensional Bi-Hamiltonian systems in chapter 4 and an integrable case (ii) Hénon-Heiles system in Chapter 5.

Another interesting development was the work of Mickens in proposing a nonstandard approach to creating discretization methods that preserve structual features [40] in which some of the rules could have been used to develop the Kahan/Hirota/Kimura scheme. This approach was used by Mickens himself to produce another discretization of the Lotka-Volterra system [39] that is similar to that of Kahan's, but used an asymmetric rule rather than a symmetric one. This has been the motivation to devise a general method for discretizing particular systems using some of these rules, and this has been done for the Lotka-Volterra system (to reproduce results already obtained by Roeger) in Chapter 3, reaction kinetics governed by the Law of Mass Action and a Hamiltonian system with a quartic potential, both in Chapter 6.

1.2 Summary of Results

In Chapter 3 a generalised discretization of the Lotka-Volterra system was presented, and although the findings of the three symplectic maps have already been presented by Roeger the method used to discover them took a different approach. By requiring that the map produced by the numerical scheme is birational before restraining it to be symplectic, a list of 7 birational maps for the Lotka-Volterra system has been generated, which were then used to reproduce the three symplectic maps. Given that the most general form of the Lotka-Volterra system is given as

$$\frac{\tilde{x}-x}{h} = ax + (1-a)\tilde{x} - (bxy + c\tilde{x}\tilde{y} + dx\tilde{y} + e\tilde{x}y), \tag{1}$$

$$\frac{\tilde{y}-y}{h} = -Ay - (1-A)\tilde{y} + Bxy + C\tilde{x}\tilde{y} + Dx\tilde{y} + E\tilde{x}y. \tag{2}$$

then the 7 birational maps are given by the following sets of parameter values:

Case (i): $\{a, b, 0, 0, 1-b, A, 0, C, 0, 1-C\}$

Case (ii): $\{a, b, 0, d, 1-b-d, A, 0, 0, 0, 1\}$

Case (iii): $\{a, 0, c, d, 1-c-d, A, 0, 0, 1, 0\}$

Case (iv): $\{a, 0, 0, d, 1-d, A, 0, 0, D, 1-D\}$

Case (v): $\{a, 0, 0, 1, 0, A, B, 0, D, 1-B-D\}$

Case (vi): $\{a, 0, 0, 0, 1, A, 0, C, D, 1-C-D\}$

Case (vii): $\{a, 0, c, 1-c, 0, A, B, 0, 1-B, 0\}$

The three symplectic maps are given by:

Case (i): $\{a, b, 0, 0, 1-b, A, 0, C, 0, 1-C\}$

Case (ii): $\{a, 0, 0, d, 1-d, A, 0, 0, d, 1-d\}$

Case (iii): $\{a, 0, c, 1-c, 0, A, B, 0, 1-B, 0\}$

This result further confirms that these three maps are the only currently known discretizations of the Lotka-Volterra system that peserve the structural properties of the original continuous system.

The key results from Chapter 4 are the presentations of three new maps created by applying the Kahan discretization to three flows found in a list of twelve presented by Gumral and Nutku [18] which are bi-Hamiltonian flows each associated with a pair of real three-dimensional Lie algebras. The Diophantine integrability test has been applied to each of these with the conclusion that none of them are likely to be integrable. The three new maps are as follows:

$$\frac{\tilde{x}-x}{\epsilon} = -\tilde{x}z - x\tilde{z}, \qquad \frac{\tilde{y}-y}{\epsilon} = -a(\tilde{y}z - y\tilde{z}), \qquad \frac{\tilde{z}-z}{\epsilon} = 2\tilde{x}x + 2a\tilde{y}y, \tag{3}$$

$$\begin{gathered} \frac{\tilde{x}-x}{\epsilon} = -\tilde{x}z - x\tilde{z}, \qquad \frac{\tilde{y}-y}{\epsilon} = -(\tilde{x}+\tilde{y})z - (x+y)\tilde{z}, \\ \frac{\tilde{z}-z}{\epsilon} = (2\tilde{x}+\tilde{y})x + (\tilde{x}+2\tilde{y})y, \end{gathered} \tag{4}$$

$$\begin{gathered} \frac{\tilde{x}-x}{\epsilon} = \tilde{x}y + (\tilde{y}-2b\tilde{x})x, \qquad \frac{\tilde{y}-y}{\epsilon} = -b\tilde{x}y - (2\tilde{x}+b\tilde{y})x, \\ \frac{\tilde{z}-z}{\epsilon} = (2\tilde{y}+b\tilde{z})x + (2\tilde{x}+2b\tilde{y}-\tilde{z})y + (b\tilde{x}-\tilde{y})z. \end{gathered} \tag{5}$$

In Chapter 5 the Hirota-Kimura/Kahan discretization method was applied to an integrable case (ii) Hénon-Heiles system which produced a discrete system that is symplectic but unfortunately does not preseve the Hamiltonians. In comparison to the Bäcklund transformation for the same system it is noted that while the Hirota-Kimura type numerical scheme produces a map lacking some of the original features, it is a much simpler method to apply and is likely to produce similar maps for other Hénon-Heiles systems.

The key results from Chapter 6 arise from applying the same method for producing general discretization schemes to two different systems. First it is applied to a reaction kinematics system with the result of confirming the only birational discretization of the system which had already been presented by Hone

[26], which is as follows:

$$\frac{\tilde{x}-x}{\epsilon} = a - cx - (1-c)\tilde{x} + x\tilde{x}\tilde{y}, \qquad \frac{\tilde{y}-y}{\epsilon} = b - x^2\tilde{y}, \tag{6}$$

where a, b, c are free parameters.

Secondly the method is applied to a Hamiltonian system with a quartic potential, with the result of producing a single map with free parameters a and b:

$$\frac{\tilde{x}-x}{h} = \tilde{p}, \qquad \frac{\tilde{p}-p}{h} = ax^3 - bx. \tag{7}$$

1.3 Continuous Dynamical Systems

A continuous dynamical system has a phase space that evolves over continuous time and can be represented by an ordinary differential equations (ODEs) or partial differential equations (PDEs). We will be looking only at ODEs. A typical first order n-dimensional system of ODEs can be given by

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}), \tag{8}$$

where $\dot{\mathbf{x}}$ represents the time derivatives of the dependent variables $\mathbf{x} = (x_1, x_2, ..., x_n)$, and the $\mathbf{F} : \mathbb{R}^n \mapsto \mathbb{R}^n$ is a vector of functions:

$$\mathbf{F}(\mathbf{x}) = \begin{pmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ . \\ . \\ f_n(\mathbf{x}) \end{pmatrix}. \tag{9}$$

It should be noted that this is an autonomous system which means that the differential equations do not depend on the independent variable t. A key feature of such continuous systems that will be important throughout this thesis is the stability of the fixed points of the system. A fixed point of an ODE is a set of coordinates in the phase space that is fixed under the time evolution of the system, and are defined as follows.

Definition 1.3.1. *A point* $\mathbf{x}^*$ *is called a fixed point, or steady state, of a continuous dynamical system (8) , if* $\mathbf{F}(\mathbf{x}^*) = 0$.

In the phase space the fixed points will be the intersections of the *nullclines* which are the sets of points that satisfy each equation $f_i(x_1, x_2, ..., x_n) = 0$ for all $i = 1, .., n$.

In order to analyse the stability of the fixed points, and therefore the behaviour of the solutions of the system, we need to define the Jacobian matrix.

Definition 1.3.2. *The Jacobian matrix, J, of a system of* ODE's *in definition 1.1.1 is a matrix of the partial derivatives of* $\mathbf{F}$ *as follows*

$$J(\mathbf{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & . \quad . \quad . & \frac{\partial f_1}{\partial x_n} \\ . \quad . & & . \\ . & . & . \\ . & \quad . & . \\ \frac{\partial f_n}{\partial x_1} & . \quad . \quad . & \frac{\partial f_n}{\partial x_n} \end{pmatrix}.$$

The Jacobian matrix is used to linearize the system of ODE's which means to approximate them using a linear system, and near the fixed points this will usually be a good enough approximation to identity the nature of the fixed point. The linear system for each fixed point is created by evaluating the Jacobian matrix at the fixed point to give the system

$$\dot{\mathbf{x}} = A\mathbf{x}, \tag{10}$$

where $A = J(\mathbf{x}^*)$ is sometimes known as the *community matrix* [42]. The eigenvalues, λ_j of the matrix A are calculated as the roots of the characteristic equation

$$\det |A - \lambda I| = 0, \tag{11}$$

where I is the $n \times n$ identity matrix. If all these eigenvalues have non-zero real parts ($Re(\lambda_j) \neq 0$, for all j) then x^* is known as a *hyperbolic* fixed point.

The linear stability analysis criteria are given as follows.

Theorem 1.3.3. (Poincare-Lyapunov). *If the eigenvalues λ_j of the Jacobian matrix evaluated at the fixed point have non-zero real parts, then the trajectories of the system around the fixed points will behave in the same way as the associated linear system. The different cases of stability are:*

(i) $\lambda_j \in \mathbb{R}$ and $\lambda_j < 0$ indicates a stable node (sink) and nearby solutions will be attracted to and end at the fixed point.

(ii) $\lambda_j \in \mathbb{C}$ and $Re(\lambda_j) < 0$ indicates a stable spiral (sink) and nearby solutions will spiral around and eventually end at the fixed point.

(iii) $\lambda_j \in \mathbb{R}$ and $\lambda_j > 0$ indicates an unstable node (source) and nearby solutions will move away from the fixed point.

(iv) $\lambda_j \in \mathbb{C}$ and $Re(\lambda_j) > 0$ indicates an unstable spiral (source) and nearby solutions will spiral away from the fixed point.

(v) $\lambda \in \mathbb{R}$ and λ_j have different signs indicates a saddle point (unstable).

In the degenerate case of $Re(\lambda_j) = 0$ (pure imaginary) the fixed point is classified as a centre, and the trajectories of the linear system will form elliptical orbits with the fixed point lying in the centre of the ellipse, which is considered stable.

See Appendix B for an example demonstrating stability analysis.

1.4 Hamiltonian Mechanics

The phase space of a canonical Hamiltonian system has even dimension $2m$ and the coordinates consist of m position variables q_i and m momentum variables p_i which are canonical coordinates. On the phase space a Hamiltonian system is specified by a function $H(q_i, p_i)$ called the Hamiltonian, and it is the partial derivatives of this function that define the time evolution of the system,

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}. \tag{12}$$

The Hamiltonian H is known as an invariant or first integral because it is conserved with time, $\frac{dH}{dt} = 0$, and in classical mechanics it is the total energy of the system (usually the sum of kinetic and potential energy). In order to consider the integrability of Hamiltonian systems we must first define Poisson brackets and symplectic forms which follows in the next section.

1.4.1 Poisson brackets

A Poisson bracket is an important operator in Hamiltonian mechanics, and to define this operator we shall let M be an n-dimensional manifold and $\mathcal{F}$ be the set of all smooth real-valued functions that are defined on M.

Definition 1.4.1. *A Poisson bracket on M is defined as a bilinear operator, denoted $\{,\} : \mathcal{F}(M) \times \mathcal{F}(M) \mapsto \mathcal{F}(M)$, such that for any $f, g, h \in \mathcal{F}$,*

(i) $\{\alpha f + \beta g, h\} = \alpha\{f, h\} + \beta\{g, h\}$, (linearity)

(ii) $\{f, g\} = -\{g, f\}$, (skew-symmetry)

(iii) $\{f, \{g, h\}\} + \{g, \{h, f, \}\} + \{h, \{f, g\}\} = 0$, (Jacobi identity)

(iv) $\{f, gh\} = g\{f, h\} + \{f, g\}h$, (Leibniz property)

for all $\alpha, \beta \in \mathbb{R}$.

The general representation of a Poisson bracket is given (using local coordinates x_i, $i = 1, ..., n$) as

$$\{f, g\} = \sum_{j,k=1}^{n} \{x_j, x_k\} \frac{\partial f}{\partial x_j} \frac{\partial g}{\partial x_k}, \tag{13}$$

When using canonical coordinates (q_i, p_i), $i = 1, ..., m$, and a manifold with dimension $n = 2m$ the Poisson bracket is represented as a special case of (13)

$$\{f, g\} = \sum_{i=1}^{m} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) \tag{14}$$

with $\{q_j, p_k\} = \delta_{jk}$.

Definition 1.4.2. *A Poisson bracket is described as nondegenerate if* $\{f, g\} = 0$ *for all* f *implies that* g *is a constant function.*

A nondegenerate Poisson bracket can only exist when n is even, and a canonical Poisson bracket will always be nondegenerate and the manifold M it is defined on will be symplectic (see section 1.5).

One last feature of a Poisson structure to mention before relating back to Hamiltonian systems is the possible existence of Casimir functions, which is only possible if the Poisson structure is degenerate.

Definition 1.4.3. *A Casimir* C *of a Poisson bracket is a non-constant function on* M*, so that* $\{C, f\} = 0$*, for all* $f \in \mathcal{F}(M)$*.*

For a canonical Hamiltonian system the equations of motion (12) can be written using the Poisson bracket (14) as follows

$$\dot{q}_i = \{q_i, H\}, \qquad \dot{p}_i = \{p_i, H\}, \tag{15}$$

where the dot denotes the time derivative. The evolution with time of any function

f on the phase space of a Hamiltonian system is defined by the Poisson bracket,

$$\dot{f} = \{f, H\}, \tag{16}$$

which leads to the fact that any Casimir function C on the phase space is also an invariant of the system (conserved with time), as $\dot{C} = \{C, H\} = 0$. Any system with an even dimension and a Poisson bracket is automatically symplectic, and therefore all Hamiltonian systems are symplectic, which also implies that they preserve phase space volume.

It is also possible for a system to exhibit two Poisson brackets, in which case the system has a bi-Hamiltonian structure. The two Poisson brackets are called compatible and are defined as follows.

Definition 1.4.4. *The Poisson brackets $\{\cdot,\cdot\}_1$ and $\{\cdot,\cdot\}_2$ are said to be compatible if*

$$\{\cdot,\cdot\}_{\mu,\lambda} = \mu\{\cdot,\cdot\}_1 + \lambda\{\cdot,\cdot\}_2,$$

i.e any linear combination, is also a Poisson bracket.

1.4.2 Integrability

In this thesis we will be taking integrability to be as defined by Liouville, who first introduced the notion of integrability in the 19th Century [5]. The notion of integrability for Hamiltonian systems is defined as follows.

Definition 1.4.5. *A Hamiltonian system $\dot{x}_i = \{x_i, H\}$ on a manifold M, dim M=2N, with a non-degenerate Poisson bracket $\{,\}$ is completely integrable in the sense of Liouville if there exist N functionally conserved quantities $F_1, ..., F_N$ which are in involution with respect to $\{\cdot,\cdot\}$, that is $\{F_j, F_k\} = 0$ for all j, k.*

When a system is integrable it is possible to integrate it in the following sense [3].

Theorem 1.4.6. (Liouville-Arnold). *The solutions to the equations of motion of a completely integrable system can be found using quadratures.*

It is clear that any two-dimensional Hamiltonian system must be completely integrable as it already possesses one conserved quantity, H.

1.4.3 Examples of Hamiltonian Systems

In this section we will give a few examples of Hamiltonian systems to demonstrate the descriptions and definitions in this chapter so far. The examples given will be in addition to the systems explored in the later chapters.

Example 1. The first example is a well known two-dimensional system called the harmonic oscillator, and in the coordinates (q, p) the Hamiltonian is given as

$$H = \frac{1}{2m}p^2 + \frac{1}{2}mw^2q^2, \tag{17}$$

where m is the mass of the particle and w is the angular frequency of the oscillator. The first term of the Hamiltonian represents the kinetic energy and the second term represents the corresponding potential energy. The equations of motion for this system are as follows.

$$\dot{q} = \{q, H\} = \frac{p}{m}, \qquad \dot{p} = \{p, H\} = -mw^2q. \tag{18}$$

Different values of the Hamiltonian correspond to ellipses in the (q, p) plane as shown in figure 1, and each value is fixed by initial conditions.

Example 2. The four-dimensional example given here is known as the two-body problem, or the Kepler problem, and it is a Hamiltonian system that describes the motion of two bodies, such as a planet and the sun. If one body is much heavier then we can take it to be the center of the coordinate system and consider it motionless, and the position of the second body is given by (q_1, q_2) with its

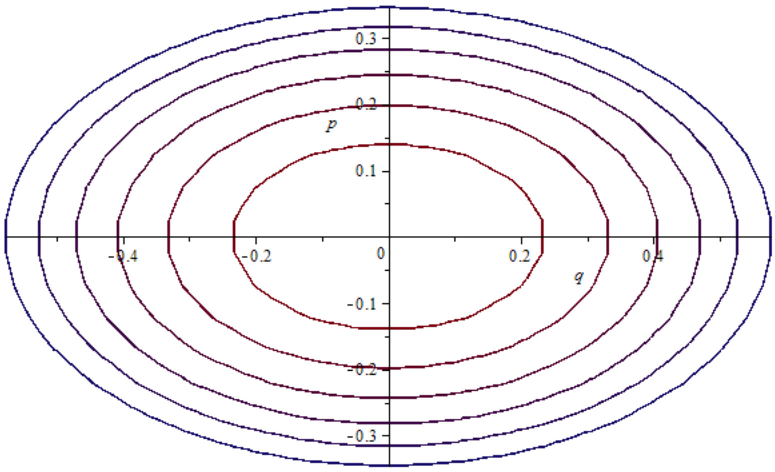

Figure 1: Orbits of the harmonic oscillator with m=0.01 and w=60.

motion restricted to the plane. The Hamiltonian for this system is as follows.

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}, \tag{19}$$

and this gives rise to the following equations of motion:

$$\dot{q_1} = p_1, \qquad \dot{q_2} = p_2, \qquad \dot{p_1} = \frac{-q_1}{(q_1^2 + q_2^2)^{\frac{3}{2}}}, \qquad \dot{p_2} = \frac{-q_2}{(q_1^2 + q_2^2)^{\frac{3}{2}}}. \tag{20}$$

As this system is four-dimensional, to be completely integrable in the sense of Liouville, it must have a second conserved quantity that is in involution with H meaning $\{H, L\} = 0$ for some function L, and in this case this second invariant is the angular momentum L as given below:

$$L = q_1 p_2 - q_2 p_1. \tag{21}$$

To confirm that this is indeed constant along any orbit we can check that it is a Casimir of the Poisson bracket:

$$\{H, L\} = \frac{q_1}{(q_1^2 + q_2^2)^{\frac{3}{2}}} \cdot (-q_2) - p_1 \cdot p_2 + \frac{q_2}{(q_1^2 + q_2^2)^{\frac{3}{2}}} \cdot q_1 - p_2 \cdot (-p_1) = 0. \tag{22}$$

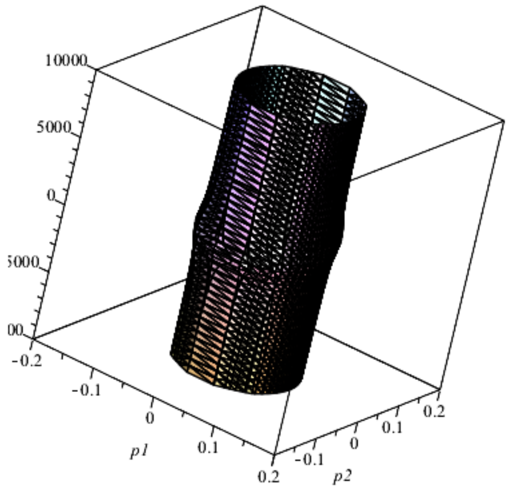

Figure 2: Invariant surface arising from the two-body system, with $h = 4 \times 10^{-3}$ and $l = 100$.

Given the two invariants H and L we can also assert that all solutions of this system are confined to the intersections of the four-dimensional surfaces $H = h$ and $L = l$, where h, l are constants determined by the initial conditions. This intersection implicitly defines a two-dimensional surface in a four-dimensional phase space, and depending on the sign of h we get two different types of surface. If $h > 0$ or $h = 0$ the surface is essentially a cylinder (figure 2), and this corresponds to the case where one of the bodies has enough energy to escape the gravitational attraction and the trajectories will wind around this surface towards positive or negative infinity. The other case $h < 0$ gives a torus (figure 3) and one would expect the generic trajectories will be quasi-periodic, and will wind around the torus without repeating themselves. However, for the Kepler problem, it can be shown that the $h < 0$ solutions always form ellipses.

1.5 Numerical Integration

Numerical integration is a process that takes a continuous dynamical system that is described by differential equations and reformulates it into a discrete dynamical

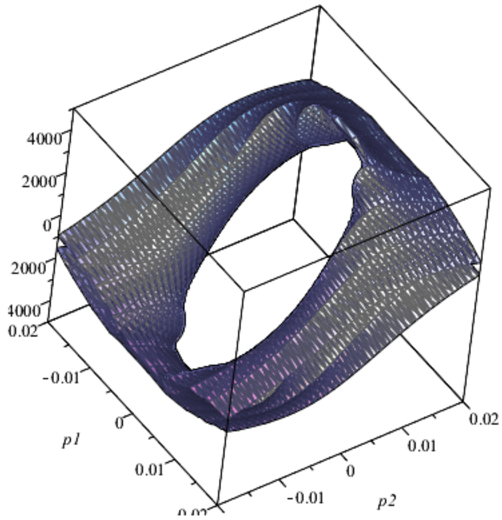

Figure 3: Invariant surface arising from the two-body system, with $h = -1.5\times10^{-4}$ and $l = 50$.

system that is described by difference equations. Numerical integration methods provide a way to find numerical approximations to the solutions of continuous dynamical systems, which is particularly useful for the many continuous systems that cannot be solved analytically.

During the process of numerical integration the continuous dependent and independent variables are replaced by discrete counterparts. The discrete independent variable can take any real or complex value whereas the discrete dependent variable is evaluated only at integer shifts of the independent variable. If we take an ODE

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}), \tag{23}$$

where $\mathbf{F}(\mathbf{x})$ is a vector of non-linear functions and define a time step to be $\Delta t = h$, a fixed real value, then the variables $(t, \mathbf{x}(t))$ are replaced as follows:

$$t \to t_n = t_0 + nh, \qquad \mathbf{x}(t) \to \mathbf{x}_n = \mathbf{x}(t_0 + nh), \tag{24}$$

with n being an integer. The function $\mathbf{F}(\mathbf{x})$ is replaced by $\mathbf{F}_n$ which is an approximation of $\mathbf{F}(x_n)$. The first derivative of $\mathbf{x}(t)$ can be approximated using the

Taylor expansion of $\mathbf{x}(t)$,

$$\mathbf{x}(t+h) = \mathbf{x}(t) + h\frac{d\mathbf{x}}{dt} + \frac{h^2}{2}\frac{d^2\mathbf{x}}{dt^2} + ... = \sum_{k=0}^{\infty} \frac{h^k}{k!}\frac{d^k\mathbf{x}}{dt^k}. \tag{25}$$

Using the notation described above we have $\mathbf{x}_1 = \mathbf{x}(t+h)$ and $\mathbf{x}_0 = \mathbf{x}(t)$, and denoting all terms involving h^2 and higher as $O(h^2)$ we have

$$\mathbf{x}(t_0+h) = \mathbf{x}(t_0) + h\frac{d\mathbf{x}(t_0)}{dt} + O(h^2). \tag{26}$$

Rearranging this gives the first derivative as:

$$\frac{d\mathbf{x}(t_0)}{dt} = \frac{\mathbf{x}(t_0+h) - \mathbf{x}(t_0)}{h} + O(h), \tag{27}$$

and the smaller the time step h the more accurate this approximation is. For any integer value n the overall difference equation that replaces the ODE (23) is

$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{h} = \mathbf{F}_n, \tag{28}$$

where $\mathbf{F}_n$ is defined by the particular method used. The replacement of the first derivative on the left hand side is known as the forward difference scheme, and $\mathbf{F}_n = \mathbf{F}(\mathbf{x}_n)$ gives the forward Euler method, one of the standard schemes mentioned in section 1.4 on standard numerical integrators.

Throughout this thesis we will use the following notation and conventions when working with discrete systems (x will be replaced by the variable/s concerned in the system being discussed).

Definition 1.5.1. Notation for difference equations.

(i) $\tilde{x}$ represents x_{n+1}, and x represents x_n.

(ii) h will always represent the step-size Δt.

(iii) x_0 will represent an initial value.

1.6 Local and Global Error

When referring to the accuracy of a numerical integrator we are actually considering the local and global error. Up to given time step in the iteration of a numerical scheme the global error is defined as the difference between the exact solution and the numerical approximation. The local error however, is the error incurred by a single step in the iteration. The smaller these errors are the more accurate the numerical integrator is at approximating the solution. However, in this thesis we are not interested in the error as such, but rather in the long term behaviour of the solutions.

1.7 Standard Numerical Integrators

The simplest numerical integrator for a typical ODE

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x})$$

is to take the forward Euler finite difference scheme as an approximation of the first derivative, and then simply replace all $\mathbf{x}$ terms in $\mathbf{F}(\mathbf{x})$ with $\mathbf{x}_n$.

$$\frac{\tilde{\mathbf{x}} - \mathbf{x}}{h} = \mathbf{F}(\mathbf{x}). \tag{29}$$

This difference equation can be rearranged to give an explicit equation for the step variable $\tilde{\mathbf{x}}$:

$$\tilde{\mathbf{x}} = h\mathbf{F}(\mathbf{x}) + \mathbf{x}. \tag{30}$$

This very basic scheme is sufficient for approximating the first few iterations, given an initial value, to a reasonable degree of accuracy. However, even with a very small time step, the orbit produced by this difference equation usually begins to wander far from the path of the trajectories of the original continuous system.

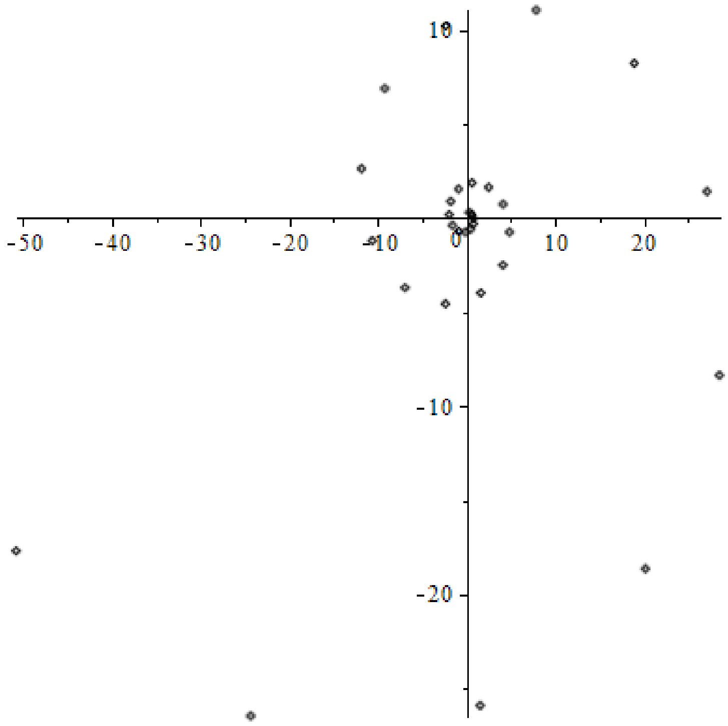

Figure 4: 30 iterations of the Euler forward difference scheme ($h = 0.01$) applied to the Harmonic Oscillator, with $m = 0.01$ and $w = 60$, and initial conditions $q_0 = p_0 = 0.3$.

This lack of conservation of qualitative behaviour can be seen very well using the first example given in the previous section. Applying this finite difference scheme to the harmonic oscillator equations of motion (18) we have the following difference equations.

$$\tilde{q} = \frac{hp}{m} + q, \qquad \tilde{p} = -hmw^2q + p. \tag{31}$$

As seen in figure 1 the orbits of the Harmonic Oscillator are closed curves (ellipses), and therefore we would expect the iterations of a discrete model of this system to also follow a closed curve in the phase space. However, as seen in figure 4 with only a few iterations the orbit is increasingly spiraling out from the initial values.

The time derivative can also be replaced with other finite difference approximations:

$$\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{h} = \mathbf{F}(\mathbf{x}_n), \tag{32}$$

$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_{n-1}}{2h} = \mathbf{F}(\mathbf{x}_n). \tag{33}$$

The first is the implicit backward Euler method, and the second is the explicit central difference method (also known as the mid-point method).

1.7.1 Multi-step Methods

Multi-step methods have been developed as they offer a better approximation to the continuous system, since they depend on more than one previous value. A generalised form of a multi-step method looks like

$$\sum_{i=0}^{k} \alpha_i x_{n+i} = h \sum_{i=0}^{k} \beta_i \mathbf{F}(\mathbf{x}_{n+i}), \tag{34}$$

where $\alpha_k = 1$ and $|\alpha_0| + |\beta_0| > 0$. These methods are implicit unless $\beta_k = 0$, and are not very useful for the preservation of the properties of the original continuous system as they need extra initial conditions, therefore creating spurious solutions.

1.7.2 Runge-Kutta Methods

This class of methods is made more accurate due to the use of more points in the single time step interval $[t_n, t_{n+1}]$ in the calculation of each iteration. A general form of a Runge-Kutta (RK) method is given as

$$\frac{x_{n+1} - x_n}{h} = \sum_{i=1}^{m} b_i k_i, \qquad k_i = F(t_n + c_i h, x_n + h \sum_{j=1}^{m} a_{ij} k_j), \tag{35}$$

where m denotes the stages of the method. A very well known and used RK method is a fourth order method (RK4) given below.

$$\frac{x_{n+1}-x_n}{h} = \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right),$$

with

$$\begin{aligned} k_1 &= F(t_n, x_n),\\ k_2 &= F(t_n + \frac{h}{2}, x_n + \frac{hk_1}{2}),\\ k_3 &= F(t_n + \frac{h}{2}, x_n + \frac{hk_2}{2}),\\ k_4 &= F(t_n + h, x_n + hk_3). \end{aligned} \tag{36}$$

In this method each iteration is a weighted average of four increments, each of which are a product of h and an estimate of the slope.

1.8 Symplectic forms and symplectic maps

Any manifold with a canonical Poisson bracket is an example of a symplectic manifold, a smooth manifold equipped with a closed differential two-form ω, called a symplectic form, defined as

$$\omega = \sum \mathrm{d}p_j \wedge \mathrm{d}q_j. \tag{37}$$

A map is said to be symplectic if it preserves the sum of areas projected onto a set of (q_i, p_i) planes, and these areas are represented by symplectic forms.

Definition 1.8.1. *A map $\phi : M \mapsto M$ on a $2N$ dimensional manifold M is symplectic if the symplectic form ω is preserved, that is $\phi^*\omega = \omega$.*

Furthermore, the condition for which a map is defined as symplectic is

$$D\phi^T P D\phi = P, \qquad P = \left(\begin{array}{cc} 0 & I \\ -I & 0 \end{array} \right), \tag{38}$$

where P is the Poisson matrix, I is the $N \times N$ identity matrix and $D\phi$ is the Jacobian of the map. For a two dimensional map ($N = 1$), the condition for the map to be symplectic is simply $\det(D\phi) = 1$.

A symplectic map has the equivalent features that a symplectic continuous system has, including invariants (conserved quantites).

Definition 1.8.2. *A function F on M is an invariant for the map ϕ if and only if*

$$F \circ \phi = \phi^* F = F$$

holds.

Integrabilty also needs to be defined for maps, and the definition for integrability in the Liouville sense can be extended to discrete systems [57].

Definition 1.8.3. *A symplectic map $\phi : M \mapsto M$ on the $2N$ dimensional manifold M is said to be integrable if it has N first integrals $f_1, f_2, ..., f_N$ in involution.*

Finding any possible first integrals (invariants) of a map can prove challenging, so we will be employing a test for integrability (Diophantine test) to assess the nature of the maps studied later in the thesis, and this test is presented in section 1.9.

It will be necessary to check that a map preserves a Poisson bracket.

Definition 1.8.4. *The map $\phi : M \mapsto M$ is said to preserve the Poisson bracket $\{\cdot, \cdot\}$ if*

$$\phi^* \{f, g\} = \{\phi^* f, \phi^* g\}$$

for all f, g.

It is worth noting that for a two dimensional symplectic map it is possible to narrow the classification of fixed points. To demonstrate this we start with a symplectic map in Darboux (canonical) coordinates.

$$\phi : \begin{pmatrix} q \\ p \end{pmatrix} \mapsto \begin{pmatrix} \tilde{q} \\ \tilde{p} \end{pmatrix} = \begin{pmatrix} F(q,p) \\ G(q,p) \end{pmatrix}. \tag{39}$$

For this map we have that the fixed points are defined by $F(q,p) = q$ and $G(q,p) = p$, and the Jacobian matrix is

$$J = \begin{pmatrix} \frac{\partial F}{\partial q} & \frac{\partial F}{\partial p} \\ \frac{\partial G}{\partial q} & \frac{\partial G}{\partial p} \end{pmatrix}. \tag{40}$$

If we then diagonalise at the fixed points of the map we get that the two eigenvalues λ_1, λ_2 satisfy $\lambda_1\lambda_2 = \det(J)$, but because we know the map is symplectic we have that $\det(J) = 1$ so $\lambda_1\lambda_2 = 1$. This gives two possibilities, one of which is that both eigenvalues are real and non-zero which implies $|\lambda_1| \geq 1$ and $|\lambda_2| \leq 1$ without loss of generality, and therefore giving a saddle point. The other possibility is that the two eigenvalues are complex conjugate pairs with modulus 1, which gives a center, [29].

We have now defined what we expect from symplectic maps (also known as canonical transformations), which we are aiming to produce using non-standard finite difference schemes later in the thesis.

1.9 Symplectic Integrators

Symplectic integrators are finite difference schemes that respects the symplectic nature of Hamiltonian dynamics, and the resulting maps will possess a Hamiltonian that is slightly perturbed from that of the original continuous system. Examples of standard symplectic integrators are the symplectic or semi-explicit

Euler methods and the implicit mid-point method, the latter of which has been covered in section 1.4, and the former will be presented in section 2.5.

For continuous systems with a Hamiltonian of the form $H(q, p) = T(p) + V(q)$ symplectic integrators can be derived using the splitting method [11].

1.10 Diophantine Test for Integrability

The criteria for the integrability of discrete equations have developed rapidly over the last few decade; for example the singularity confinement property of Grammaticos, Ramani and Papageorgiou has resulted in the discovery of many integrable discrete equations [17]. However, not all of these criteria have been sufficient to detect integrability alone, and in the case of singularity confinement Hietarinta and Viallet [20] found non-integrable equations that possess this property, showing that further criteria are needed to fully determine integrability. The additional concept that Hietarinta and Viallet introduced is that of algebraic entropy as a measure of degree growth, and the idea that, for an integrable equation, the degree of the n^{th} iterate as a rational function of the initial conditions grows no faster than a polynomial in n is something that a number of authors have been studying [58, 4, 20].

The algebraic entropy approach has a related numerical test that is much quicker to use as a detector of integrability, as presented by Halburd in [19].The measure of growth is achieved by analysing the *heights* of the iterates over the discrete time evolution.

Definition 1.10.1. *The height H of a rational nonzero number $x = \frac{s}{t} \in \mathbb{Q}$ is $H(x) = \max \{|s|, |t|\}$, where s, t have no common factors and $H(0) = 1$.*

Definition 1.10.2. Diophantine integrability (Halburd). *A polynomial discrete equation, $y_{n+1} = f(y_n)$, is Diophantine integrable if the logarithmic height of its iterates, $h(y_n) = \log H(y_n)$, grows no faster than a polynomial in n.*

The concept of using this property as a measure of complexity comes from a similarity between the definitions and theorems of Diophantine approximation and Nevanlinna theory, observed by Osgood [45] and independently 'translated' by Vojta [59] to produce a dictionary between the two areas. For difference equations Diophantine integrability is the natural analogue of the Painleve property for ODE's [9].

1.11 Outline of Thesis

We now give an outline of the contents of the rest of the chapters in this thesis.

Chapter 2 presents non-standard numerical schemes that have already been discovered, including a method that was first noted by Kahan in 1993 in a set of lecture notes [32], and then presented again by Hirota and Kimura in 2000 applied to the Euler top system [21]. We also present a set of rules devised by Mickens [40] that if followed are expected to produce discrete systems with very desirable features, an example of which Mickens applied to the Lotka-Volterra system in 2003 [39]. These non-standard schemes have been reported to preserve features of various continuous systems but sometimes it is unclear as to exactly why they work so well.

In Chapter 3 the 2-dimensional Lotka-Volterra system is presented along with known non-standard discretizations applied to it. We then go on to find a generalised scheme that creates a discrete analogue of the Lotka-Volterra system that is birational and symplectic, and therefore preserves the fixed points and their stability. Three different cases for the parameters involved are discovered by looking at the constraints on the most general version of the system given when we require birationality and then symplecticity. These cases are identical to those presented by Roeger in [52] although they were discovered using a different method.

Chapter 4 looks at 3-dimensional Bi-Hamiltonian systems and starts by presenting the Hirota-Kimura discretization of the Euler top. We then go on to look at 3-dimensional flows from a list of 12 presented by Gümral and Nutku [18], nine of which have been discretized using the Kahan scheme by Hone and Petrera [27]. The remaining three are then presented and the Diophantine test for integrability is applied.

In Chapter 5 the focus is on the Hénon-Heiles system, and in particular the integrable case (ii) which is presented through the reduction of the fifth order KdV equation. The Hirota-Kimura/Kahan method is then applied and through a numerical example we see that the elliptic fixed point of the original system is preserved. This discretization is briefly compared to the Bäcklund transformation for the Hénon-Heiles case (ii).

Finally in Chapter 6 a general non-standard discretization of a trimolecular system is investigated and although no new discretizations are discovered, the method used does confirm that those given in [40] are indeed the only birational possibilities. A Hamiltonian system with a quartic potential is then looked at in the second part of the chapter and the same method for finding the general discretization is used and then the Diophantine integrability test is used to conclude that the discrete system is in fact not Diophantine integrable.

Chapter 2

Non-standard Numerical Integration Methods

2.1 The Hirota-Kimura Discretization/Kahan's Method

In 1993 a set of lectures was delivered by Kahan in which he proposed a new method for discretizing an ODE $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ where the function $\mathbf{f}(\mathbf{x})$ is a polynomial of degree two in the components $x_1, x_2, ..., x_n$ of the vector $\mathbf{x}$. The difference equation formed as a result of applying Kahan's method is of the form

$$\frac{\tilde{\mathbf{x}} - \mathbf{x}}{h} = \mathbf{Q}(\tilde{\mathbf{x}}, \mathbf{x}), \tag{41}$$

where $\mathbf{Q}(\tilde{\mathbf{x}}, \mathbf{x})$ is a quadratic function that is defined by the rule (42) below. The time derivative has been replaced by the usual Euler forward difference, and the terms of the polynomial are each replaced according to a symmetric rule as follows:

$$\dot{x}_j \mapsto \frac{\tilde{x}_j - x_j}{h}, \quad x_j x_k \mapsto \frac{x_j \tilde{x}_k + \tilde{x}_j x_k}{2}, \quad x_j \mapsto \frac{x_j + \tilde{x}_j}{2}, \quad c \mapsto c. \tag{42}$$

On first inspection this scheme appears to be implicit; however, as the right hand side is linear in each $\tilde{x_j}$ and x_j equation (41) can be solved explicitly to find $\tilde{\mathbf{x}}$ as a rational function of $\mathbf{x}$ and vice versa. This means that Kahan's scheme produces a birational map $\phi : \mathbf{x} \mapsto \tilde{\mathbf{x}}$, which can be written explicitly [32] as:

$$\phi : \tilde{\mathbf{x}} = \mathbf{x} + h\left(\mathbf{I} - \frac{h}{2}\mathbf{f}'(\mathbf{x})\right)^{-1}\mathbf{f}(\mathbf{x}), \qquad \left(\mathbf{I} - \frac{h}{2}\mathbf{f}'(\mathbf{x})\right)^{-1}\mathbf{f}(\mathbf{x}) = \mathbf{Q}(\tilde{\mathbf{x}}, \mathbf{x}), \quad (43)$$

where $\mathbf{I}$ is the $n \times n$ identity matrix and $\mathbf{f}'$ is the Jacobian of $\mathbf{f}$. The inverse of this map is

$$\phi^{-1} : \mathbf{x} = \tilde{\mathbf{x}} - h\left(\mathbf{I} + \frac{h}{2}\mathbf{f}'(\tilde{\mathbf{x}})\right)^{-1}\mathbf{f}(\tilde{\mathbf{x}}), \quad (44)$$

It has already been proven by Roegers that Kahan's method produces a discrete map with the same fixed points possessing the same local stability as the original continuous system. If the fixed point of the original system is $\mathbf{x}^*$ then it holds that

$$\phi(\mathbf{x}^*) = \mathbf{x}^*, \quad (45)$$

and taking the derivative of the map at the fixed point we have

$$\phi' : \mathbf{x}^* = \mathbf{I} + h\left(\mathbf{I} - \frac{h}{2}\mathbf{f}'(\mathbf{x}^*)\right)^{-1}\mathbf{f}'(\mathbf{x}^*). \quad (46)$$

For each eigenvalue of the original system we have a corresponding eigenvalue $\mu(h)$ of (46):

$$\mu(h) = \frac{1 + \frac{h\lambda}{2}}{1 - \frac{h\lambda}{2}}, \quad (47)$$

where λ represents an eigenvalue of the original system.

2.2 Mickens' Method and its Modifications

In 1994 Mickens wrote a book [40] in which he presents rules for the construction of non-standard finite-difference schemes. These rules are as follows:

- **Rule 1**: The orders of the discrete derivatives must be exactly equal to the orders of the corresponding derivatives of the differential equations.
- **Rule 2**: Denominator functions for the discrete derivatives must, in general, be expressed in terms of more complicated functions of the step-sizes than those conventionally used.
- **Rule 3**: Nonlinear terms must, in general, be modeled non-locally on the computational grid or lattice.
- **Rule 4**: Special solutions of the differential equations should also be special (discrete) solutions of the finite-difference models.
- **Rule 5**: The finite-difference equations should not have solutions that do not correspond exactly to solutions of the differential equations.

Although these rules will not always result in the creation of an exact finite-difference scheme, Mickens suggests that the discrete systems produced will possess very desirable properties.

Later, in 2003, Mickens presented a non-standard discretization of the Lotka-Volterra system, [39], that produces a map that preserves the qualities of the solutions of the original system. In creating this scheme Mickens used the rules outlined above, to give the following discrete Lotka-Volterra system:

$$\frac{\tilde{x}-x}{\sin(h)} = 2x - \tilde{x} - \tilde{x}y, \qquad \frac{\tilde{y}-y}{\sin(h)} = -\tilde{y} + 2\tilde{x}y - \tilde{x}\tilde{y}. \tag{48}$$

This map has the same qualities as the continuous Lotka-Volterra system (which will be studied in more detail in the next chapter):

$$\frac{dx}{dt} = x(1-y), \qquad \frac{dy}{dt} = y(x-1). \tag{49}$$

It can be seen that the derivatives of these differential equations have been approximated by modified forward Euler expressions and therefore have the same order (Rule 1), and that they have been modified by the replacement of the denominator h with $\sin(h)$, such that the denominator function $\phi(h) = h + O(h^2)$ (Rule 2). Rule 3 has been enforced by ensuring that each term on the right hand side of the differential equations is modeled non-locally, for example meaning that x cannot simply be replaced with x_n or x_{n+1}, but it must be expressed as $2x - \tilde{x}$ so that it can be modeled using both x_n and x_{n+1}. Mickens does not give the reasons as to why these replacements work, but the numerical evidence is clear that this map produces the same periodic solutions as the continuous system.

2.2.1 Modifications

In 2004 Mounim and de Dormale [41] presented two numerical methods for the Lotka-Volterra system as modifications of Micken's method (48), with a claim that they produce more accurate numerical solutions. These two modified methods are created by enforcing the condition that the discrete system has the symmetry property that the right-hand sides of (49) has. The discrete equivalent of this property is that the right-hand sides of the discrete system should transform to each other under the interchanges $x \leftrightarrow y$ and $n \leftrightarrow \tilde{n}$.

Modified scheme 1:

$$\frac{\tilde{x} - x}{\phi(h)} = x - 2\tilde{x}y - xy, \qquad \frac{\tilde{y} - y}{\phi(h)} = -\tilde{y} + 2\tilde{x}y - \tilde{x}\tilde{y}. \tag{50}$$

Modified scheme 2:

$$\frac{\tilde{x} - x}{\phi(h)} = 2x - \tilde{x} - \tilde{x}y, \qquad \frac{\tilde{y} - y}{\phi(h)} = -2\tilde{y} + y - \tilde{x}y. \tag{51}$$

2.3 The Symplectic Euler method

In [16] Gander and Meyer-Spasche presented a symplectic version of Euler's method restricted to two dimensional canonical Hamiltonian systems. Given a two dimensional canonical Hamiltonian system with a separable Hamiltonian $H(p,q) = f(p) + g(q)$,

$$\dot{q} = \frac{\partial H(p,q)}{\partial p} = H_p(p,q), \qquad \dot{p} = -\frac{\partial H(p,q)}{\partial q} = -H_q(p,q) \tag{52}$$

the symplectic Euler method is presented as

$$\frac{\tilde{q}-q}{h} = H_p(\tilde{p},q), \qquad \frac{\tilde{p}-p}{h} = -H_q(p,q). \tag{53}$$

Gander and Meyer-Spasche then go on to define the symplectic Euler method for the two dimensional non-canonical Hamiltonian system: the Lotka-Volterra system, which using the same notation and variables as the previous section (with all parameters set to 1) is presented as

$$\frac{\tilde{x}-x}{h} = x - xy, \qquad \frac{\tilde{y}-y}{h} = -y + \tilde{x}y. \tag{54}$$

Chapter 3

General discretizations of the Lotka-Volterra system

3.1 The Lotka-Volterra System

The Lotka-Volterra system models the behaviour of various populations which can have different types of interaction with each other. The 2-dimensional Lotka-Volterra system we will be looking at in this paper is the predator-prey interaction of two species [23, 22, 42]. The most general form of this system of first order differential equations is shown in (55) where $u(\tau)$ represents the population of the prey, and $v(\tau)$ represents the predator, and of course a, b, c and d are positive constants.

$$\frac{du}{d\tau} = u(a - bv), \qquad \frac{dv}{d\tau} = v(cu - d), \tag{55}$$

To give the simplest and most general form of this system we can non-dimensionalise to reduce the four parameters to just one parameter. To do this we start with the change of variables $u = \lambda x, v = \mu y, \tau = \nu t$ and then choose the values $\nu = \frac{1}{a}, \mu = \frac{a}{b}, \lambda = \frac{a}{c}$ which gives the system

$$\frac{dx}{dt} = x(1-y), \qquad \frac{dy}{dt} = y(x-\alpha), \tag{56}$$

where $\alpha = \frac{d}{a}$ is the only parameter, and in this chapter I will be looking at this system with $\alpha = 1$. It is well known that this system is a Hamiltonian system which we can see by the following change of variables:

$$x = e^q, \qquad y = e^p \tag{57}$$

Substituting these new variables into the system (56) with $\alpha = 1$ gives the new system:

$$\dot{q} = 1 - e^p, \qquad \dot{p} = e^q - 1. \tag{58}$$

This system now satisfies Hamilton's equations:

$$\dot{p} = \frac{\partial H}{\partial q}, \qquad \dot{q} = -\frac{\partial H}{\partial p}, \tag{59}$$

with the Hamiltonian $H = e^q + e^p - q - p$.

The system (56) with $\alpha = 1$ also features a Poisson bracket and invariant volume form which are given below:

$$\{x, y\} = xy, \tag{60}$$

$$\omega = d\log(x) \wedge d\log(y) = \frac{1}{xy} dx \wedge dy. \tag{61}$$

This system exhibits two fixed points, $(0,0)$ and $(1,1)$ and linear stability analysis can be used to show the nature of these. The Jacobian of the system,

$$J = \begin{pmatrix} 1-y & -x \\ y & x-1 \end{pmatrix}, \tag{62}$$

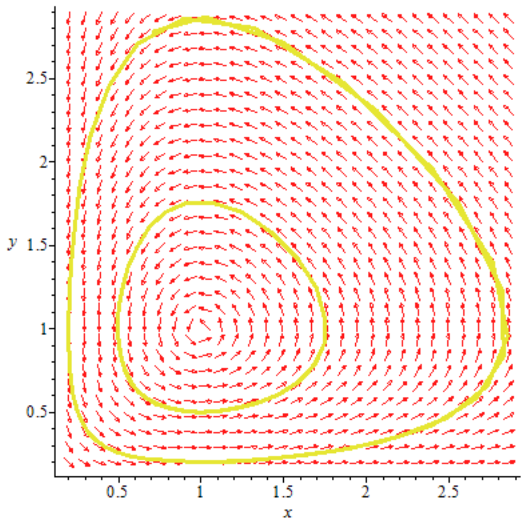

Figure 5: The phase portrait of (56) with $\alpha = 1$ showing two closed curve solutions created using initial conditions $x_0 = 0.5, y_0 = 1$ and $x_0 = 1, y_0 = 0.2$.

evaluated at each of the fixed points gives the following eigenvalues:

$$(0,0) \to \lambda_1 = 1, \lambda_2 = -1, \qquad (1,1) \to \lambda_1 = i, \lambda_2 = -i, \tag{63}$$

which indicate a saddle point at $(0,0)$ and a centre at $(1,1)$. The phase portrait of this system clearly shows that the solutions lie on closed level curves of the Hamiltonian $H(x,y) = x + y - \ln(x) - \ln(y)$.

It is because this system has closed solutions in the phase space that there is difficulty in obtaining the correct behaviour in numerical solutions of discretizations of it. Slight perturbations in the right hand side of the equations (56) can cause solutions to spiral in or out rather than follow closed orbits.

3.2 Known Non-standard schemes

For this particular system there have been a few discretizations which have been shown to preserve the qualitative features of the original continuous system and also to hold the property of being symplectic (area-preserving). These discretizations are (using the notation $\tilde{x} = x_{n+1}$, $x = x_n$ and h is the time step):

1) **The Kahan or Hirota-Kimura type discretization:** [27]

$$\frac{\tilde{x}-x}{h}=\frac{1}{2}\left(\tilde{x}+x-\tilde{x}y-x\tilde{y}\right), \qquad \frac{\tilde{y}-y}{h}=\frac{1}{2}\left(\tilde{x}y+x\tilde{y}-\tilde{y}-y\right) \tag{64}$$

2) **The Mickens type discretization:** [39]

$$\frac{\tilde{x}-x}{\sin(h)}=2x-\tilde{x}-\tilde{x}y, \qquad \frac{\tilde{y}-y}{\sin(h)}=-\tilde{y}+2\tilde{x}y-\tilde{x}\tilde{y}, \tag{65}$$

3) **Two modified Euler type discretizations:**

$$\frac{\tilde{x}-x}{h}=x(1-y), \qquad \frac{\tilde{y}-y}{h}=y(\tilde{x}-1), \tag{66}$$

$$\frac{\tilde{x}-x}{h}=x(1-\tilde{y}), \qquad \frac{\tilde{y}-y}{h}=y(x-1). \tag{67}$$

The aim of this chapter is to look at the most general form of a discretization for this system and check for which values of the parameters the discretization preserves the features of the original system, and which parameter families the above discretizations fall into. This generalised discretization will take the form

$$\frac{\tilde{x}-x}{h}=F_1(x,y,\tilde{x},\tilde{y}), \qquad \frac{\tilde{y}-y}{h}=F_2(x,y,\tilde{x},\tilde{y}). \tag{68}$$

The particular properties which we are looking for in the discretization are as follows:

i) Birationality, meaning that each of the equations in (68) can be solved explicitly to not only find rational functions for $\tilde{x}$ and $\tilde{y}$, but also for x and y. The advantage of having an explicit method and its inverse is that the system can be integrated forwards or backwards in time.

ii) The iteration plot of the discretization has the same qualitative features as the original system. In this case we are looking for closed loops in the positive quadrant of the xy-plane, even with reasonably large values of the time step ($h > 0.1$).

iii) The discrete system has the same fixed points and stability as the original system. For this example we are looking for two fixed points $(0, 0)$ and $(1, 1)$, with $(0, 0)$ as a saddle point, and $(1, 1)$ as a centre.

iv) Preservation of the symplecticity of the original system. Further details of how to check this condition are found in section 3.5.

3.3 Roeger's result

In 2006 Roeger presented a class of nonstandard symplectic numerical methods for the Lotka-Volterra systems [52] based on conditions defined by Mickens [40]. This result is presented here for comparison later in this Chapter.

The Lotka-Volterra system in [52] is defined as

$$\frac{dx}{dt} = Ax + Bxy, \qquad \frac{dy}{dt} = Cy + Dxy, \tag{69}$$

and using the notation $x_n = x$ and $x_{n+1} = X$ the general numerical method before Micken's conditions are applied takes the form

$$\frac{X-x}{h} = A(a_1x + a_2X) + B(b_1xy + b_2Xy + b_3xY + b_4XY),$$
$$\frac{Y-y}{h} = C(c_1y + c_2Y) + D(d_1xy + d_2Xy + d_3xY + d_4XY), \quad (70)$$

where $a_1 + a_2 = 1$, $c_1 + c_2 = 1$, $b_1 + b_2 + b_3 + b_4 = 1$ and $d_1 + d_2 + d_3 + d_4 = 1$.

Roeger finds three classes for the discretization of the xy terms, with the linear term parameters $a_1 = 1 - a_2$, $c_1 = 1 - c_2$ being free. These three classes are

$$(b_1xy + b_2Xy + b_3xY + b_4XY, d_1xy + d_2Xy + d_3xY + d_4XY) =$$

$$\text{Class I:} \quad (\beta xy + (1-\beta)Xy, (1-\alpha)Xy + \alpha XY), \quad (71)$$

$$\text{Class II:} \quad (\beta Xy + (1-\beta)xY, \beta Xy + (1-\beta)xY), \quad (72)$$

$$\text{Class III:} \quad (\beta xY + (1-\beta)XY, (1-\alpha)xy + \alpha xY). \quad (73)$$

3.4 A general form of a Non-standard Discrete Lotka-Volterra map

To make the most general discretization for this Lotka-Volterra system we need to include all combinations of the variables $x, y, \tilde{x}, \tilde{y}$ as the discrete equivalent of the xy terms in (56). This gives us the following 10-parameter discretization:

$$\frac{\tilde{x}-x}{h} = ax + (1-a)\tilde{x} - (bxy + c\tilde{x}\tilde{y} + dx\tilde{y} + e\tilde{x}y), \quad (74)$$

$$\frac{\tilde{y}-y}{h} = -Ay - (1-A)\tilde{y} + Bxy + C\tilde{x}\tilde{y} + Dx\tilde{y} + E\tilde{x}y. \quad (75)$$

and with the requirement that this is a first order method we have the condition

$$b + c + d + e = B + C + D + E = 1. \tag{76}$$

In order to neatly present the final cases of general discretizations these 10 parameters will be presented as

$$(a, b, c, d, e, A, B, C, D, E) \tag{77}$$

with the consideration that only 8 of these parameters are independent due to condition (76).

Now we need to look at the restrictions for this particular system, and firstly we require that it should be birational. Straight away we can see that if we solve one of the equations for one of the variables, x say, and substitute this into the other equation we will have a quadratic equation for one of the variables and therefore upon solving we have two possible solutions. This formulates some constraints on the parameters in order to produce only one solution. If we take a general quadratic equation,

$$p_2 x^2 + p_1 x + p_0 = 0, \tag{78}$$

then we have two possibilities for this equation to give one solution, the first of which is to set $p_2 = 0$ leaving a linear equation with solution $x = \frac{-p_0}{p1}$. Secondly we can set $p_0 = 0$ which leaves the equation $x(p_2 x + p_1) = 0$ and if we assume $x = 0$ cannot be a solution then we have the single solution $x = \frac{-p_1}{p_2}$.

There is also the more general case to consider in which the quadratic (78) has two rational roots where either only one of the roots is valid or there is a repeated root. This would require the discriminant $p_1^2 - 4p_2p_0$ to equal a perfect square or zero respectively. This case is discussed further in [28], and although it does produce conditions for the parameters it does not produce any new constraints beyond what is discovered from the previous two possibilities. Therefore the equations produced by this case will not be presented.

So now we have various different routes to go down to produce different constraints on this general discretization, which should give us a few different parameter families which are all birational. The first routes we shall explore are those which involve only solving for $\tilde{x}$ and x at first and then looking at the quadratic formed in $\tilde{y}$ and y respectively. Then we can look at solving for $\tilde{y}$ and y first and looking at the quadratic in $\tilde{x}$ and x respectively. There are also the two other combinations of these, one is to solve for $\tilde{x}$ and y first, and the other is to solve for $\tilde{y}$ and x first.

- **Solving for $\tilde{x}$ and x first**

Firstly (75) is solved for $\tilde{x}$ and this is then substituted into (74) which gives a quadratic equation for $\tilde{y}$. The coefficient of the squared term in this equation set to zero is given below.

$$(-cDh^2 + Cdh^2)x + c(h + Ah^2 - h^2) = 0 \tag{79}$$

Looking at the coefficient of x and the constant term separately we have the two constraints

$$-cD + Cd = 0, \tag{80}$$

$$c(1 + Ah - h) = 0. \tag{81}$$

From the second constraint (81) we have that $c = 0$ as we cannot have $A = \frac{h-1}{h}$ as we require the parameters to be independent of h. Substituting $c = 0$ into the first constraint (80) we have two possibilities, either $C = 0$ or $d = 0$. We are not quite finished finding the constraints for this route however as we also need to look at solving for the unshifted variable x also. So solving (74) for x and substituting this into (75) we are presented with a quadratic equation for y. Again taking the coefficient of the squared term and setting it to zero we have:

$$(-Bh^2d + h^2Cb - Bh^2c + Bh^2 + h^2Db - h^2b)\tilde{x} - hb + Ah^2b = 0 \qquad (82)$$

Again looking at the coefficient of $\tilde{x}$ and the constant term separately we have the constraints

$$(C + D - 1)b - B(c + d - 1) = 0 \qquad (83)$$

$$(-1 + Ah)b = 0 \qquad (84)$$

Here the second constraint (84) gives us $b = 0$ as of course we cannot have $A = \frac{1}{h}$. Substituting this into the other constraint (83) gives two options again, either $B = 0$ or $c + d = 1 \Rightarrow d = 1$ as $c = 0$.

Therefore this route has given us in total three 4-parameter families which are listed below:

1) $c = C = 0$, $b = 0$ and $B = 0$ which leaves $\{A, a, D, d\}$ as the free parameters.

2) $c = C = 0$, $b = 0$ and $d = 1$ which leaves $\{A, a, B, D\}$ as the free parameters.

3) $c = 0$, $d = 0$, $b = 0$ and $B = 0$ which leaves $\{A, a, C, D\}$ as the free parameters.

We can also look at the other possible routes, where we take the constant term to be zero and assume that the variable in question cannot equal zero as a solution. So if we take the same constraints (80) and (81) but then when solving for x we take the constant term equal to zero in the quadratic equation for y.

This gives us the following equation:

$$
\begin{aligned}
&(-h^2d + dh + h^2Ad + D\tilde{x}h^2c - C\tilde{x}h^2d)\tilde{y}^2 + \\
&(-1 + h - Ah - Ah^2a + h^2a + \tilde{x}h^2Ca - \tilde{x}h^2D - ha + \tilde{x}hC + \tilde{x}h^2Da + \tilde{x}hD)\tilde{y} = 0.
\end{aligned} \tag{85}
$$

This equation gives more constraints which are listed below:

$$Dc - Cd = 0, \tag{86}$$

$$d(1 - h + hA) = 0, \tag{87}$$

$$D(1 - h + ah) + C(1 + ah) = 0, \tag{88}$$

$$(Ah - 1)(ah - h + 1) = 0. \tag{89}$$

Now we can see that we can have choices of the parameters which will satisfy the first three constraints (86), (87) and (88), however the last constraint (89) cannot be solved as we cannot have either $A = \frac{1}{h}$ or $a = \frac{h-1}{h}$. Therefore we gain no new families of discretizations from this route.

Another route to consider is when we are solving for $\tilde{x}$ and this time we take the constant term to be zero in the quadratic equation for $\tilde{y}$. This route gives the following constraints:

$$b(1 - C - D) - B(1 - c - d) = 0, \tag{90}$$

$$(1 - Ah)(b + c + d + 1) = 0, \tag{91}$$

$$(1 + ah)(C + D - 1) + Bh = 0, \tag{92}$$

$$(Ah - 1)(ah - h + 1) = 0. \tag{93}$$

This route also brings us to a dead end as we have the same constraint (93) as we did before (89) so it is not possible to satisfy all of these constraints. So from solving for $\tilde{x}$ and x first we have found three 4-parameter families of birational discretizations.

As we have seen we cannot get any more families from setting the constant term in the quadratic equation to zero, and this continues to be the case for all the other possible routes, so from now we will just look at setting the squared term to zero.

- **Solving for $\tilde{y}$ and y first**

The next routes to inspect are those starting with solving for $\tilde{y}$ and y, which gives the following constraints:

$$c(1-B-D)-C(1-b-d)=0, \tag{94}$$

$$C(ah+1-h)=0, \tag{95}$$

$$Bd-bD=0, \tag{96}$$

$$B(1+ah)=0. \tag{97}$$

Solving all 4 of these constraints at once gives another three 4-parameter families which are given below:

4) $c=C=0$, $b=0$ and $B=0$ which leaves $\{A,a,D,d\}$ as the free parameters.

5) $c=C=0$, $B=0$ and $D=0$ which leaves $\{A,a,b,d\}$ as the free parameters.

6) $C = 0$, $B = 0$, $D = 1$ and $b = 0$ which leaves $\{A, a, c, d\}$ as the free parameters.

Clearly family 4) is exactly the same as family 1) found through the previous routes, so we have only gained two new families, bringing the running total now to five 4-parameter families.

- **Solving for $\tilde{y}$ and x first**

This route provides the following constraints:

$$c(1 - B - D) - C(1 - b - d) = 0, \tag{98}$$

$$C(ah + 1 - h) = 0, \tag{99}$$

$$(C + D - 1)b - B(c + d - 1) = 0, \tag{100}$$

$$(-1 + Ah)b = 0. \tag{101}$$

Again solving these constraints we have the following 4-parameter families arising:

7) $c = C = 0$, $b = 0$ and $B = 0$ which leaves $\{A, a, D, d\}$ as the free parameters.

8) $c = C = 0$, $b = 0$ and $d = 1$ which leaves $\{A, a, B, D\}$ as the free parameters.

9) $C = 0$, $b = 0$, $D = 1$ and $B = 0$ which leaves $\{A, a, c, d\}$ as the free parameters.

10) $C = 0$, $b = 0$, $B + D = 1$ and $c + d = 1$ which leaves $\{A, a, B, c\}$ as the free parameters.

Here 10) is the only new family giving six families in total.

- **Solving for $\tilde{x}$ and y first**

This final route provides the following constraints:

$$-cD + Cd = 0, \tag{102}$$

$$c(1 + Ah - h) = 0, \tag{103}$$

$$Bd - bD = 0, \tag{104}$$

$$B(1 + ah) = 0. \tag{105}$$

Again solving these constraints we have the following 4-parameter families arising:

11) $c = C = 0$, $B = 0$ and $b = 0$ which leaves $\{A, a, D, d\}$ as the free parameters.

12) $c = C = 0$, $B = 0$ and $D = 0$ which leaves $\{A, a, b, d\}$ as the free parameters.

13) $c = 0$, $B = 0$, $d = 0$ and $b = 0$ which leaves $\{A, a, C, D\}$ as the free parameters.

14) $c = 0$, $B = 0$, $d = 0$ and $D = 0$ which leaves $\{A, a, C, b\}$ as the free parameters.

We only have one new family, which is family 14), bringing the total number of 4-parameter families to seven which is a final total as we have now explored all possible routes.

For all families of the birational discretization we have that A and a are always free as they are in Roeger [52] ,and then the remaining paramters fit into one of the following cases, which have been presented as the following theorem using the notation (77):

Theorem 3.4.1. *The system (74),(75) is a birational discretization of the Lotka-Volterra system (56) with $\alpha = 1$ if and only if the parameters belong to one of the following cases:*

$$\text{Case (i): } \{a, b, 0, 0, 1-b, A, 0, C, 0, 1-C\}$$
$$\text{Case (ii): } \{a, b, 0, d, 1-b-d, A, 0, 0, 0, 1\}$$
$$\text{Case (iii): } \{a, 0, c, d, 1-c-d, A, 0, 0, 1, 0\}$$
$$\text{Case (iv): } \{a, 0, 0, d, 1-d, A, 0, 0, D, 1-D\}$$
$$\text{Case (v): } \{a, 0, 0, 1, 0, A, B, 0, D, 1-B-D\}$$
$$\text{Case (vi): } \{a, 0, 0, 0, 1, A, 0, C, D, 1-C-D\}$$
$$\text{Case (vii): } \{a, 0, c, 1-c, 0, A, B, 0, 1-B, 0\}$$

We can see that the four discretizations outlined in the introduction all fit into one or more of these cases. The Hirota-Kimura type discretization (64) falls under case (iv) only with $\{d, D\}$ as the extra free parameters. Micken's method (65) falls under both cases (i) and (vi), as this method just requires C to be free (apart from the replacement of h with $\sin(h)$). The first modified Euler method (66) falls under either case (i) or (ii), requiring b to be a free parameter, and the second modified Euler method (67) fits into case (v) or (vii), with B as a free parameter.

3.5 General symplectic discretizations of the Lotka-Volterra system

We know that the four methods defined in the introduction are all symplectic but this does not imply that all members of the family which they fall under are also symplectic. The way to check if a discretization is symplectic is to confirm whether or not the area form for the continuous system is preserved under the time step. The area form for the continuous Lotka-Volterra system is shown below.

$$\Omega = \frac{1}{xy} dx \wedge dy \tag{106}$$

For (106) to be preserved with each time step we need the following equation to be satisfied:

$$d\tilde{x} \wedge d\tilde{y} = \frac{\tilde{x}\tilde{y}}{xy} dx \wedge dy, \tag{107}$$

This is equivalent to

$$\det(J) - \frac{\tilde{x}\tilde{y}}{xy} = 0, \tag{108}$$

where J is the Jacobian of the system:

$$J = \begin{pmatrix} \frac{\partial \tilde{x}}{\partial x} & \frac{\partial \tilde{x}}{\partial y} \\ \frac{\partial \tilde{y}}{\partial x} & \frac{\partial \tilde{y}}{\partial y} \end{pmatrix} \tag{109}$$

Performing this calculation for the seven bi-rational maps found in the last section, only two cases are symplectic without further restrictions on the parameters, which are case (i) and case (vii). All of the other cases become symplectic with an extra condition on the parameters. To find these extra conditions we look for factorisations of the parameters in the left hand side of equation (108). For example, the equation (108) applied to case (ii) yielded the following after factorisation:

$$\frac{-d(xyh^2)f}{g} = 0 \tag{110}$$

where f, g are functions of (x, y, h, A, a, b, d). From this we can clearly see adding the constraint $d = 0$ we satisfy this equation, therefore case (ii) is symplectic with

$d = 0$. The new list of cases which are birational and also symplectic are shown below:

$$\textbf{Symplectic Case (i)} : \{a, b, 0, 0, 1-b, A, 0, C, 0, 1-C\}$$
$$\textbf{Symplectic Case (ii)} : \{a, b, 0, 0, 1-b, A, 0, 0, 0, 1\}$$
$$\textbf{Symplectic Case (iii)} : \{a, 0, c, 1-c, 0, A, 0, 0, 1, 0\}$$
$$\textbf{Symplectic Case (iv)} : \{a, 0, 0, d, 1-d, A, 0, 0, d, 1-d\}$$
$$\textbf{Symplectic Case (v)} : \{a, 0, 0, 1, 0, A, B, 0, 1-B, 0\}$$
$$\textbf{Symplectic Case (vi)} : \{a, 0, 0, 0, 1, A, 0, C, 0, 1-C\}$$
$$\textbf{Symplectic Case (vii)} : \{a, 0, c, 1-c, 0, A, B, 0, 1-B, 0\}$$

We find here that case (vi) and case (v) are the inverses of each other, as are case (ii) and case (iii).Also, case (ii) falls under case (i) with the added condition of $C = 0$. Similarly, (v) under (vii), with the added condition of $c = 0$. Therefore we only have three cases left, two with four free parameters and one with only three:

Theorem 3.5.1. *The system (74,75) is a symplectic bi-rational discretization of the Lotka-Volterra system (56) with $\alpha = 1$ if and only if the parameters belong to one of the following cases:*

$$\text{Case (i): } \{a, b, 0, 0, 1-b, A, 0, C, 0, 1-C\}$$
$$\text{Case (ii): } \{a, 0, 0, d, 1-d, A, 0, 0, d, 1-d\}$$
$$\text{Case (iii): } \{a, 0, c, 1-c, 0, A, B, 0, 1-B, 0\}$$

In [52] Roeger presented a method that leads to these same three cases by first requiring that the maps are symplectic, and the resulting maps happened to also be birational.

Due to the way the most general discretization (74), (75), was formulated it will always have the fixed points $(0, 0)$ and $(1, 1)$, and as these cases are all symplectic it is given that their fixed points will be either saddles or centers (as explained in section 1.5 of Chapter 1) and therefore they automatically preserve the stability of the original Lotka-Volterra system. An example to denomstrate this is given in section 3.6.

3.6 Stability Analysis

We will take case (i) with parameter values $A = a = 0.5, C = b = 1$ as a particular example. Using these values for the free parameters we can look at the stability of the two fixed points and we expect to find a saddle point at $(0,0)$ and a center at $(1,1)$, and given these stability conditions we would also expect the iteration plot of this particular system to represent the original system almost perfectly, even with fairly large values of h and many iterations.

First we look at the fixed point $(0,0)$, and to analyse the stability of this fixed point we first need to look at the Jacobian evaluated at $(0,0)$, which happens to be exactly the same for all of the symplectic families of discretizations listed above when keeping all the parameters free. So we have

$$J(0,0) = \begin{pmatrix} \frac{1+ah}{1+ah-h} & 0 \\ 0 & \frac{1-Ah}{1+h-Ah} \end{pmatrix} \tag{111}$$

where the diagonal entries are the eigenvalues as the matrix is diagonal. For this particular system with $A = a = 0.5$ we have the eigenvalues:

$$\lambda_1 = \frac{1+0.5h}{1-0.5h}, \qquad \lambda_2 = -\frac{1-0.5h}{1+0.5h}. \tag{112}$$

From these eigenvalues it is clear that this fixed point is a saddle point as $|\lambda_1| > 1$ and $|\lambda_2| < 1$. Now we just need to check the second fixed point, $(1,1)$ which has a more complicated Jacobian, shown below for this particular system:

$$J(1,1) = \begin{pmatrix} \frac{1+ah}{1} & \frac{2h}{h-2} \\ -\frac{2h}{h-2} & -\frac{3h^2+4h-4}{h^2-4h+4} \end{pmatrix}. \tag{113}$$

To find the eigenvalues we find the characteristic equation $\det(J - \lambda I) = 0$ where I is the identity matrix, then we solve for λ which gives:

$$\lambda_1 = -\frac{h^2 + 4h - 4 - 4\sqrt{h^3 - h^2}}{h^2 - 4h + 4}, \qquad \lambda_2 = -\frac{h^2 + 4h - 4 + 4\sqrt{h^3 - h^2}}{h^2 - 4h + 4}, \tag{114}$$

and as $h^3 < h^2$ for $h < 1$ we have two complex eigenvalues which are conjugate to each other. This is typical of a center in a discrete system, which is exactly what we were looking for. Now that we have confirmed that the fixed points have exactly the same stability as the original system the last property to confirm is that this system preserves the qualitative features of the system. Figure 6 shows the iteration plot for this map with initial conditions $x_0 = 0.1, y_0 = 1$, 10000 iterations and a step size of $h = 0.1$, and as expected we appear to have a close loop as in the original system.

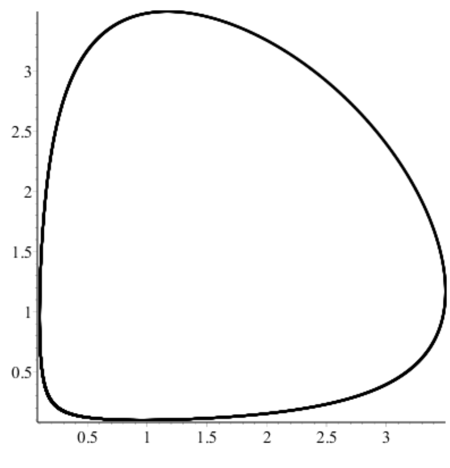

Figure 6: The iteration plot of a particular example of Case (i) with initial conditions $x_0 = 0.1, y_0 = 1$ and $h = 0.1$.

If we compare this plot with an iteration plot using a case (ii) discretization without the extra parameter conditions to make it symplectic, as in figure 7, we can see that this system preserves the features of the original Lotka-Volterra system but only for the first few iterations, and then it quickly begins to spiral towards the fixed point and therefore no longer has the correct stability of the fixed point $(1, 1)$.

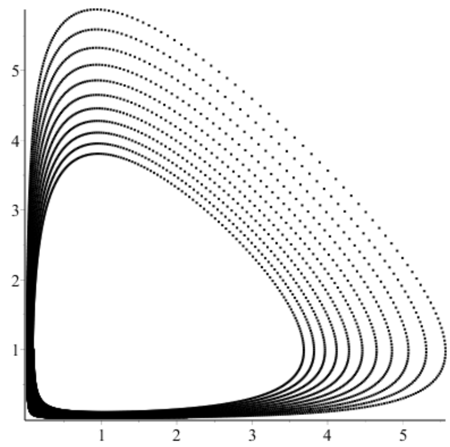

Figure 7: The iteration plot of a particular example of case (ii) with initial conditions $x_0 = 0.1, y_0 = 1$ and $h = 0.1$.

3.7 Conclusion

In this Chapter we have reproduced the three symplectic maps derived by Roeger, [52], using a different approach and therefore also producing a list of seven birational maps for the Lotka-Volterra system. We began with a generalised form of the discrete Lotka-Volterra map that included every combination of the variables $x, y, \tilde{x}, \tilde{y}$ for the quadratic term in the continuous system, which featured 10 parameters (8 independent) that we then looked for constraints for. Rather than beginning this parameter reduction by requiring that the map is symplectic, we took the approach of enforcing birationality to produce the parameter constraints. Future work on this would include applying this generalised discretization method to other systems with quadratic vector fields to build up a library of birational and symplectic discrete systems produced using this Mickens style approach.

Chapter 4

Discretizations of 3-dimensional Bi-Hamiltonian systems

In this chapter the Hirota-Kimura or Kahan discretization method is applied to three-dimensional bi-Hamiltonian systems, starting with an overview of the case of the Euler top, which was published by Hirota and Kimura [21] and provides a new integrable discrete analogue of the system. Next, a bi-Hamiltonian flow associated with a pair of real three-dimensional Lie algebras is presented and shown to have its properties preserved under the Hirota-Kimura discretization. This flow came from a list of twelve presented by Gumral and Nutku [18], and is one of the nine that were analysed under the Hirota-Kimura discretization by Hone and Petrera [27]. A further three flows from the same list not considered in [27], having one transcendental invariant alongside a rational one, are subjected to the Hirota-Kimura discretization and the properties of the resulting maps are investigated. Finally these new discretizations of the three-dimensional bi-Hamiltonian flows will be tested using the Diophantine integrability test presented by Halburd in [19].

4.1 The Euler top

4.1.1 The Continuous System

The Euler top is a well known bi-Hamiltonian system of differential equations that describe the motion of a rigid body with a fixed centre of mass [24]

$$\dot{x} = \alpha_1 yz, \qquad \dot{y} = \alpha_2 zx, \qquad \dot{z} = \alpha_3 xy, \tag{115}$$

with α_i being the parameters of the system. This system possesses two functionally independent integrals of motion, which are in involution with respect to a Poisson bracket, and has an explicit solution in terms of elliptic functions. The quadratic function $H = \beta_1 x^2 + \beta_2 y^2 + \beta_3 z^2$ is an integral of motion subject to a restriction on the parameters β_i:

$$2\beta_1 x\dot{x} + 2\beta_2 y\dot{y} + 2\beta_3 z\dot{z} = 2(\alpha_1\beta_1 + \alpha_2\beta_2 + \alpha_3\beta_3)xyz,$$

so that

$$\alpha_1\beta_1 + \alpha_2\beta_2 + \alpha_3\beta_3 = 0.$$

More precisely, the following three functions are invariant under these equations:

$$\begin{aligned} K_1 &= \alpha_3 y^2 - \alpha_2 z^2, \\ K_2 &= \alpha_1 z^2 - \alpha_3 x^2, \\ K_3 &= \alpha_2 x^2 - \alpha_1 y^2, \end{aligned} \tag{116}$$

although only two of them are functionally independent as $\alpha_1 K_1 + \alpha_2 K_2 + \alpha_3 K_3 = 0$.

It can be noted that the invariants H and K_i are related in the following way:

$$\alpha_i H = \beta_k K_j - \beta_j K_k,$$

where (i, j, k) are permutations of $(1, 2, 3)$. The Poisson bracket related to this system is given below, with $\lambda = (\lambda_1, \lambda_2, \lambda_3)^T \in \mathbb{R}^3$:

$$\{x, y\} = \lambda_1 z, \qquad \{y, z\} = \lambda_2 x, \qquad \{z, x\} = \lambda_3 y,$$

and for the system to be Hamiltonian with respect to this Poisson bracket we have a restriction on the parameters involved:

$$\dot{x} = \{x, H\} = \frac{\partial H}{\partial y}\{x, y\} + \frac{\partial H}{\partial z}\{x, z\},$$

$$\alpha_1 yz = 2\beta_2\lambda_3 yz - 2\beta_3\lambda_2 yz, \qquad \Rightarrow \alpha_1 = 2(\beta_2\lambda_3 - \beta_3\lambda_2),$$

and similar calculations give the other two constraints:

$$\alpha_2 = 2(\beta_3\lambda_1 - \beta_1\lambda_3), \qquad \alpha_3 = 2(\beta_1\lambda_2 - \beta_2\lambda_1).$$

4.1.2 The Hirota-Kimura discretization

The discretization of (115) that was presented in [21] reads as

$$\begin{aligned} \tilde{x} - x &= \epsilon\alpha_1(\tilde{y}z + y\tilde{z}), \\ \tilde{y} - y &= \epsilon\alpha_2(\tilde{x}z + x\tilde{z}), \\ \tilde{z} - z &= \epsilon\alpha_2(\tilde{x}y + y\tilde{x}). \end{aligned} \tag{117}$$

Solving (117) for $\tilde{\mathbf{x}}$ gives the map $f : \mathbf{x} \mapsto \tilde{\mathbf{x}}$ as defined by

$$\tilde{\mathbf{x}} = f(\mathbf{x}, \epsilon) = A^{-1}(\mathbf{x}, \epsilon)\mathbf{x}, \tag{118}$$

with the matrix A given by

$$A(\mathbf{x},\epsilon) = \begin{pmatrix} 1 & -\epsilon\alpha_1 z & -\epsilon\alpha_1 y \\ -\epsilon\alpha_2 z & 1 & -\epsilon\alpha_2 x \\ -\epsilon\alpha_3 y & -\epsilon\alpha_3 x & 1 \end{pmatrix}$$

The details of the features of this map (such as integrals of motion and an invariant volume form) are given in [48].

4.2 Gümral and Nutku examples

In [18] Gumral and Nutku present a list of all of the non-trivial three-dimensional bi-Hamiltonian flows, meaning that each system has two compatible Poisson tensors, P and Q, that are associated with the two independent integrals of motion, H and K. Using this notation, H is the Casimir for P, and K is the Casimir for Q, and the vector field, $\dot{\mathbf{x}} = V$ is described as

$$V = -PdH = -\frac{1}{c}QdK,$$

with c being the conformal factor. These flows also preserve a volume form which also features c:

$$\Omega = c \quad dx \wedge dy \wedge dz.$$

Hone and Petrera presented the Hirota-Kimura or Kahan discretization of nine of the twelve flows found in [18], along with two independent integrals of motion and an invariant volume form related to each map in [27]. Explicit solutions in terms of elliptic or elementary functions were also found for these maps. The first six of these flows all had non-transcendental invariants, one of which will be recalled along with the H-K discretization and the features of the new map. The last two flows featured one transcendental invariant, and three more of these type of flows will be investigated in the next section.

Throughout this chapter the vector $\mathbf{x} = (x_1, x_2, x_3)$ represents the system coordinates (x, y, z).

4.2.1 The Continuous Flow

To demonstrate the Hirota-Kimura discretization preserving the features of a continuous three-dimensional bi-Hamiltonian flow an example from [27] will now be presented. The flow reads as

$$\dot{x} = -x^2, \qquad \dot{y} = -xy, \qquad \dot{z} = 2y^2 + xz. \tag{119}$$

There are two conserved quantities for (119) as follows:

$$H = \frac{y}{x}, \qquad K = xz + y^2. \tag{120}$$

The two Poisson brackets of the system, which define the Poisson tensors P and Q respectively are defined by

$$\{x_j, x_k\}_1 = \epsilon_{jkl}\phi\frac{\partial K}{\partial x_l}, \qquad \{x_j, x_k\}_2 = \epsilon_{jkl}\psi\frac{\partial H}{\partial x_l}, \tag{121}$$

where ϵ_{jkl} is the anti-commuting symbol and the two functions of the local coordinates ϕ, ψ are yet to be determined. The equations of motion can also be written in terms of these Poisson brackets:

$$\dot{\mathbf{x}} = \{\mathbf{x}, H\}_1 = \{\mathbf{x}, K\}_2. \tag{122}$$

This relation can be used to find the two functions ϕ, ψ, and therefore express the Poisson tensors purely in terms of the system variables. Starting with the first

Poisson bracket that defines P we have the following:

$$\dot{x} = \frac{\partial H}{\partial y}\{x,y\}_1 + \frac{\partial H}{\partial z}\{x,z\}_1 = \left(\frac{1}{x}\right)\phi x = \phi = -x^2.$$

The first equation of motion indicates that the function $\phi = -x^2$ so now we just need to check this for the other two equations of motion.

$$\dot{y} = \frac{\partial H}{\partial x}\{y,x\}_1 + \frac{\partial H}{\partial z}\{y,z\}_1 = \left(\frac{-y}{x^2}\right)(-\phi x) = -xy,$$

$$\dot{z} = \frac{\partial H}{\partial x}\{z,x\}_1 + \frac{\partial H}{\partial y}\{z,y\}_1 = \left(\frac{-y}{x^2}\right)(2\phi y) - \left(\frac{1}{x}\right)\phi z = 2y^2 + xz.$$

Clearly having $\phi = -x^2$ satisfies all of the equations of motion when defined by the first Poisson bracket, and therefore we can now write down the Poisson tensor P as follows:

$$P = \begin{pmatrix} 0 & -x^3 & 2x^2y \\ x^3 & 0 & -x^2z \\ -2x^2y & x^2z & 0 \end{pmatrix} \tag{123}$$

The Poisson tensor Q is defined by the second Poisson bracket which satisfies the following first equation of motion.

$$\dot{x} = \frac{\partial K}{\partial y}\{x,y\}_2 + \frac{\partial K}{\partial z}\{x,z\}_2 = x\left(\frac{-\psi}{x}\right) = -\psi = -x^2.$$

This shows that $\psi = x^2$ so now this just needs to be checked for the other equations of motion.

$$\dot{y} = \frac{\partial K}{\partial x}\{y,x\}_2 + \frac{\partial K}{\partial z}\{y,z\}_2 = x\left(\frac{-\psi y}{x^2}\right) = -xy,$$

$$\dot{z} = \frac{\partial K}{\partial x}\{z,x\}_2 + \frac{\partial K}{\partial y}\{z,y\}_2 = z\left(\frac{\psi}{x}\right) + 2y\left(\frac{\psi y}{x^2}\right) = y^2 + xz.$$

The second Poisson bracket Q is defined below.

$$Q = \begin{pmatrix} 0 & 0 & -x \\ 0 & 0 & -y \\ x & y & 0 \end{pmatrix} \tag{124}$$

To define the volume form for this particular system it is necessary to find c, the conformal factor, which can be achieved by requiring that the volume form is preserved and solving the resulting equation.

$$\dot{\Omega} = \dot{c} dx \wedge dy \wedge dz + c[d\dot{x} \wedge dy \wedge dz + dx \wedge d\dot{y} \wedge dz + dx \wedge dy \wedge d\dot{z}] = 0,$$

$$(\dot{c} - 2cx)(dx \wedge dy \wedge dz) = 0.$$

Solving $\dot{c} = 2cx$ we have $c = \frac{1}{x^2}$ up to an overall constant and therefore a fully defined volume form $\Omega = \frac{1}{x^2} dx \wedge dy \wedge dz$.

Now that the Poisson structure of this map has been fully defined it is interesting to look at the features of the two Casimir functions. It is easy to see that H and K are preserved under the map (119), which is expected as they are the integrals of motion for the system:

$$\frac{dH}{dt} = \frac{\dot{y}}{x} + \frac{\dot{x}y}{x^2} = \frac{-xy}{x} - \frac{(-x^2 y)}{x^2} = -y + y = 0,$$

$$\frac{dK}{dt} = x\dot{z} + \dot{x}z + 2y\dot{y} = 2xy^2 + x^2 z - x^2 z - 2xy^2 = 0.$$

Both of these invariants define a surface when set equal to a constant, and the intersection of these surfaces gives a curve which is a solution trajectory of the system. Setting H equal to a constant gives a plane, and setting K to a constant gives a hyperboloid.

4.2.2 The Discretization

The Hirota-Kimura (Kahan) discretization applied to the flow (119) reads as (note that $h = 2\epsilon$)

$$\frac{\tilde{x} - x}{\epsilon} = -2\tilde{x}x, \qquad \frac{\tilde{y} - y}{\epsilon} = -\tilde{x}y - x\tilde{y}, \qquad \frac{\tilde{z} - z}{\epsilon} = 4\tilde{y}y + \tilde{x}z + x\tilde{z}, \tag{125}$$

which given in matrix form is

$$\tilde{\mathbf{x}} = A(\tilde{\mathbf{x}};\epsilon)\mathbf{x}, \qquad A = \begin{pmatrix} 1 - 2\epsilon\tilde{x} & 0 & 0 \\ -\epsilon\tilde{y} & 1 - \epsilon\tilde{x} & 0 \\ \epsilon\tilde{z} & 4\epsilon\tilde{y} & 1 + \epsilon\tilde{x} \end{pmatrix}.$$

To get the equations in the explicit form $\tilde{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ the matrix A is inverted and the following replacements are made: $\tilde{\mathbf{x}} \mapsto \mathbf{x}$ and $\epsilon \mapsto -\epsilon$.

$$\tilde{\mathbf{x}} = A(\tilde{\mathbf{x}};\epsilon)\mathbf{x} = A^{-1}(\mathbf{x};-\epsilon)\mathbf{x},$$

giving the following explicit formulae for the map:

$$\begin{aligned} \tilde{x} &= \tfrac{x}{1+2\epsilon x}, \\ \tilde{y} &= \tfrac{y}{1+2\epsilon x}, \\ \tilde{z} &= -\tfrac{3\epsilon xz + 4\epsilon y^2 + z}{(\epsilon x - 1)(1+2\epsilon x)}. \end{aligned} \tag{126}$$

In order to show that the properties of the continuous system have been preserved we now need to show that the map possesses two conserved quantities, which will be denoted $\hat{H}$ and $\hat{K}$, that are equal to the invariants (120) of the original system multiplied by a correction factor. It is clear to see from (126) that the invariant H from the continuous system will be conserved under the discrete time step, that is

$$H(\tilde{x}, \tilde{y}) = \frac{\tilde{y}}{\tilde{x}} = \frac{y}{x} = H(x, y),$$

and therefore we have that $\hat{H} = H = \frac{y}{x}$. Hone and Petrera [27] give the second conserved quantity $\hat{K}$ in terms of the second original invariant K and it reads as

$$\hat{K} = \frac{K}{1 - \epsilon^2 x^2} = \frac{xz + y^2}{1 - \epsilon^2 x^2},$$

which is shown to be conserved under the map by showing that the following holds:

$$(\tilde{x}\tilde{z} + \tilde{y}^2)(1 - \epsilon^2 x^2) = (xz + y^2)(1 - \epsilon^2 \tilde{x}^2).$$

Substituting the expressions for $\tilde{x}, \tilde{y}$ and $\tilde{z}$ into the above equation and simplifying gives

$$\frac{(xz + y^2 + 3\epsilon xy^2 + 3\epsilon x^2 z)(1 + \epsilon x)}{(1 + 2\epsilon x)^2} = \frac{(1 + 4\epsilon x + 3\epsilon^2 x^2)(xz + y^2)}{(1 + 2\epsilon x)^2},$$

of which the numerators are equal if the brackets are expanded. Therefore it is confirmed that $\hat{K}$ as defined above is indeed a conserved quantity of this map.

It is also necessary to show that the discretization has a volume form that is also preserved by the map, which is denoted $\hat{\Omega}$ and is related to Ω, the volume form of the continuous system, and the two invariants H and K.

$$\hat{\Omega} = \frac{\Omega}{HK} = \frac{1}{xy(y^2 + xz)} dx \wedge dy \wedge dz. \tag{127}$$

To show that this is preserved under the map we need to show the following holds:

$$d\tilde{x} \wedge d\tilde{y} \wedge d\tilde{z} = \frac{\tilde{x}\tilde{y}(\tilde{x}\tilde{z} + \tilde{y}^2)}{xy(xz + y^2)} dx \wedge dy \wedge dz.$$

This is equivalent to

$$\mathbf{det}\left(\frac{\partial \tilde{\mathbf{x}}}{\partial \mathbf{x}}\right) - \frac{\tilde{x}\tilde{y}(\tilde{x}\tilde{z} + \tilde{y}^2)}{xy(xz + y^2)} = 0,$$

and we have that

$$\mathbf{det}\left(\frac{\partial\tilde{\mathbf{x}}}{\partial\mathbf{x}}\right)=\frac{1}{(1+2\epsilon x)^2}\left(\frac{1+3\epsilon x}{(1-\epsilon x)(1+2\epsilon x)^2}\right).$$

Substituting in the expressions for $\tilde{x},\tilde{y},\tilde{z}$ into the right hand side we have

$$\frac{\tilde{x}\tilde{y}(\tilde{y}^2+\tilde{x}\tilde{z})}{xy(y^2+xz)}=\frac{1}{xy(xz+y^2)}\left(\frac{xy(1+3\epsilon x)(xz+y^2)}{(1-\epsilon x)(1+2\epsilon x)^4}\right).$$

Therefore it is clear that both sides of the equation are equal, and therefore the volume form $\hat{\Omega}$ is indeed preserved under the map.

Finally, to show that this discrete map is also completely integrable, two compatible Poisson tensors need to be found which will be similarly denoted $\hat{P}$ and $\hat{Q}$ that are defined by the Poisson brackets

$$\{x_j,x_k\}_1=\epsilon_{jkl}\hat{\phi}\frac{\partial\hat{K}}{\partial x_l},\qquad\{x_j,x_k\}_2=\epsilon_{jkl}\hat{\psi}\frac{\partial\hat{H}}{\partial x_l}\tag{128}$$

respectively. The two functions $\hat{\phi},\hat{\psi}$ are very closely related to the equivalent functions in the continuous set up with an extra factor to counteract the alteration to the Casimir function $\hat{K}$:

$$\hat{\phi}=(1-\epsilon^2x^2)\phi,\qquad\hat{\psi}=(1-\epsilon^2x^2)\psi.$$

Therefore the discrete Poisson brackets (128) define the following Poisson tensors for this system:

$$\hat{P}=\begin{pmatrix}0&-x^3&2x^2y\\x^3&0&\frac{-x^2z(1+\epsilon^2x^2)-2\epsilon^2x^2y^2}{(1-\epsilon^2x^2)}\\-2x^2y&\frac{x^2z(1+\epsilon^2x^2)+2\epsilon^2x^2y^2}{(1-\epsilon^2x^2)}&0\end{pmatrix},\tag{129}$$

$$\hat{Q} = \begin{pmatrix} 0 & 0 & -x(1-\epsilon^2 x^2) \\ 0 & 0 & -y(1-\epsilon^2 x^2) \\ x(1-\epsilon^2 x^2) & y(1-\epsilon^2 x^2) & 0 \end{pmatrix}. \tag{130}$$

4.3 New examples of discretizations

For the following examples the two Poisson brackets will be represented by $\{,\}_i^*$ and $\{,\}_i^{**}$, which define the Poisson tensors P_i, Q_i respectively, with $i \in \{1,2,3\}$. These brackets will take the form

$$\{x_j, x_k\}_i^* = \epsilon_{jkl}\phi_i \frac{\partial K_i}{\partial x_l}, \qquad \{x_j, x_k\}_i^{**} = \epsilon_{jkl}\psi_i \frac{\partial H_i}{\partial x_l},$$

with H_i, K_i being the two Casimir functions. The volume forms will be represented in a similar way, all with a distinct conformal factor,

$$\Omega_i = c_i dx \wedge dy \wedge dz.$$

4.3.1 The Continuous Systems

The first example, flow ξ_1, reads as

$$\xi_1 : \qquad \dot{x} = -xz, \qquad \dot{y} = -ayz, \qquad \dot{z} = x^2 + ay^2, \tag{131}$$

where a is a constant, and the two integrals of motion for this system are

$$H_1 = x^2 + y^2 + z^2, \qquad K_1 = x^{-a}y. \tag{132}$$

Note that strictly the second invariant K_1 is only transcendental when $a \notin \mathbb{Q}$, otherwise it is algebraic. Moreover, if $a \in \mathbb{Z}$ then K_1 is rational, and if $a \in \mathbb{Q}\backslash\mathbb{Z}$ then a power of K_1 will be rational. The trajectories of the system can be shown by the intersection of the sphere defined by H and the surface of section $y = Kx^a$

and the system has two possible sets of steady states depending on the sign of a. To find the steady states the following equations need to be satisfied:

$$\dot{x} = -xz = 0, \qquad \dot{y} = -ayz = 0, \qquad \dot{z} = x^2 + ay^2 = 0, \tag{133}$$

and when $a > 0$ the third equation requires that $x = y = 0$ and therefore z is free to take any value, say k_1. However when these values are substituted into H_1 we can define the steady state values in terms of a fixed value of $H > 0$.

$$H_1 = x^2 + y^2 + z^2 = 0 + 0 + k_1^2, \quad \Rightarrow \quad k_1 = \pm\sqrt{H_1}.$$

$$\mathbf{x}_{1,2}^* = (0, 0, \pm\sqrt{H_1})^T.$$

When $a < 0$ we still have the two fixed points defined above, but the third equation in (133) now has more solutions. If we let $x = \alpha_1$ then we have

$$x^2 = -ay^2, \quad \Rightarrow \quad y = \pm\frac{\alpha_1}{\sqrt{-a}},$$

and we therefore require that $z = 0$. To eliminate the need for the parameter α_1 we can again use the invariant H_1 such that

$$H_1 = \alpha_1^2 + \frac{\alpha_1^2}{-a}, \quad \Rightarrow \quad \alpha_1 = \pm\sqrt{\frac{aH_1}{a-1}},$$

to give the extra stationary points

$$\mathbf{x}_{3,4}^* = \left(\pm\sqrt{\frac{aH_1}{a-1}}, \pm\sqrt{\frac{aH_1}{a(1-a)}}, 0\right)^T.$$

As with the flow (119) this system also has a Poisson structure with the brackets and by performing similar calculations as before we can define the following functions:

$$c_1 = x^{-(a+1)}, \qquad \phi_1 = x^{a+1}, \qquad \psi_1 = \frac{-x^{a+1}}{2}.$$

Using this we can define the two Poisson tensors and preserved volume form as

$$P_1 = \begin{pmatrix} 0 & 0 & x \\ 0 & 0 & ay \\ -x & -ay & 0 \end{pmatrix}, \qquad Q_1 = x^{a+1} \begin{pmatrix} 0 & z & -y \\ -z & 0 & x \\ y & -x & 0 \end{pmatrix}$$

$$\Omega_1 = \frac{1}{x^{a+1}} dx \wedge dy \wedge dz.$$

The second example, flow ξ_2, reads as

$$\xi_2 : \qquad \dot{x} = -xz, \qquad \dot{y} = -z(x+y), \qquad \dot{z} = x^2 + xy + y^2, \tag{134}$$

and the two integrals of motion for this system are

$$H_2 = x^2 + y^2 + z^2, \qquad K_2 = \frac{y}{x} - \log x. \tag{135}$$

Again the trajectories of the system are the intersection between a sphere defined by H_2 and a surface with section defined by $y = x(K + \log x)$. The steady states of this system are found by solving the equations

$$-xz = 0, \qquad -z(x+y) = 0, \qquad x^2 + xy + y^2 = 0,$$

which gives only two possible solutions

$$\mathbf{x}^*_{1,2} = (0, 0, \pm\sqrt{H_2})^T.$$

The third example, flow ξ_3, reads as

$$\xi_3: \qquad \dot{x} = x(y - bx), \qquad \dot{y} = -x(x + by), \qquad \dot{z} = 2y(x + by) + z(bx - y), \tag{136}$$

where b is a constant, and the two integrals of motion for this system are

$$H_3 = xz + y^2, \qquad K_3 = \varphi^{(1+ib)}\varphi^{(\bar{1}-ib)}, \tag{137}$$

where $\varphi = x + iy$.

4.3.2 The Discrete maps

Applying the Hirota-Kimura type discretization to flow ξ_1 gives a map, $d\xi_1$, that reads as

$$d\xi_1: \qquad \frac{\tilde{x} - x}{\epsilon} = -\tilde{x}z - x\tilde{z}, \qquad \frac{\tilde{y} - y}{\epsilon} = -a(\tilde{y}z - y\tilde{z}), \qquad \frac{\tilde{z} - z}{\epsilon} = 2\tilde{x}x + 2a\tilde{y}y, \tag{138}$$

which written in matrix form gives

$$\tilde{\mathbf{x}} = A_1(\tilde{\mathbf{x}}; \epsilon)\mathbf{x}, \qquad A_1 = \begin{pmatrix} 1 - \epsilon\tilde{z} & 0 & -\epsilon\tilde{x} \\ 0 & 1 - a\epsilon\tilde{z} & -a\epsilon\tilde{y} \\ 2\epsilon\tilde{x} & 2a\epsilon\tilde{y} & 1 \end{pmatrix}. \tag{139}$$

Applying the Hirota-Kimura type discretization to flow ξ_2 gives a map, $d\xi_2$, that reads as

$$\begin{aligned} d\xi_2: \qquad \frac{\tilde{x} - x}{\epsilon} &= -\tilde{x}z - x\tilde{z}, \qquad \frac{\tilde{y} - y}{\epsilon} = -(\tilde{x} + \tilde{y})z - (x + y)\tilde{z}, \\ \frac{\tilde{z} - z}{\epsilon} &= (2\tilde{x} + \tilde{y})x + (\tilde{x} + 2\tilde{y})y, \end{aligned} \tag{140}$$

which written in matrix form gives

$$\tilde{\mathbf{x}} = A_2(\tilde{\mathbf{x}};\epsilon)\mathbf{x}, \qquad A_2 = \begin{pmatrix} 1-\epsilon\tilde{z} & 0 & -\epsilon\tilde{x} \\ -\epsilon\tilde{z} & 1-\epsilon\tilde{z} & -\epsilon(\tilde{x}+\tilde{y}) \\ \epsilon(2\tilde{x}+\tilde{y}) & \epsilon(\tilde{x}+2\tilde{y}) & 1 \end{pmatrix}. \tag{141}$$

The flow $d\xi_3$ reads as

$$\begin{aligned} d\xi_3: \qquad \frac{\tilde{x}-x}{\epsilon} &= \tilde{x}y + (\tilde{y}-2b\tilde{x})x, \qquad \frac{\tilde{y}-y}{\epsilon} = -b\tilde{x}y - (2\tilde{x}+b\tilde{y})x, \\ \frac{\tilde{z}-z}{\epsilon} &= (2\tilde{y}+b\tilde{z})x + (2\tilde{x}+2b\tilde{y}-\tilde{z})y + (b\tilde{x}-\tilde{y})z, \end{aligned} \tag{142}$$

which written in matrix form gives

$$\tilde{\mathbf{x}} = A_3(\tilde{\mathbf{x}};\epsilon)\mathbf{x}, \quad A_3 = \begin{pmatrix} 1+\epsilon(\tilde{y}-2b\tilde{x}) & \epsilon\tilde{x} & 0 \\ -\epsilon(2\tilde{x}+b\tilde{y}) & 1-b\epsilon\tilde{x} & 0 \\ \epsilon(2\tilde{y}+b\tilde{z}) & \epsilon(2\tilde{x}+4b\tilde{y}-\tilde{z}) & 1+\epsilon(b\tilde{x}-\tilde{y}) \end{pmatrix}. \tag{143}$$

The Diophatine integrability test has been applied to each of these systems below and it is clear that all of them have growth of the heights of their iterates greater than that of a polynomial, which indicates that the discrete systems are not integrable.

4.4 Conclusion

In this Chapter we have considered three-dimensional bi-Hamiltonian systems that originally appeared in a list produced by Gumral and Nutku [18]. In [27] Hone and Petrera present the Hirota-Kimura discretizations of six of these systems, all of which are algebraically integrable, and all of which provide maps that admit two independent rational integrals of motion. These six discrete maps have been shown to be Diophantine integrable, and one of these maps has been presented in

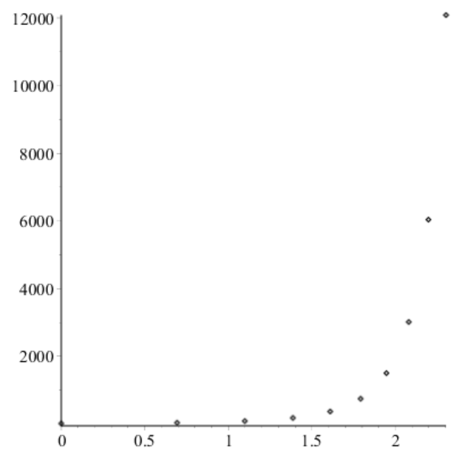

Figure 8: A plot of the growth of the heights of the iterates of x for the map in (138).

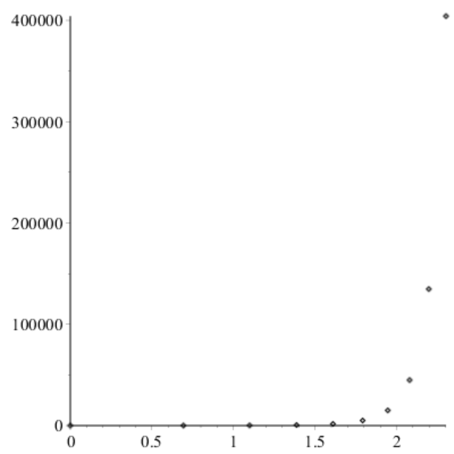

Figure 9: A plot of the growth of the heights of the iterates of x for the map in (140) .

this Chapter for comparison against three Hirota-Kimura maps that arised from continuous systems that have one rational and one transcendental integral. We find that when the Hirota-Kimura discretization is applied to a continuous system that features a transcendental integral the map produced is not integrable, unlike the case when both integrals are rational.

Further work here would include deriving the Poisson structures and volume forms for the two flows ξ_2 and ξ_3, and also to find the corresponding discrete Poisson structures for all three maps. It would also be interesting to investigate further

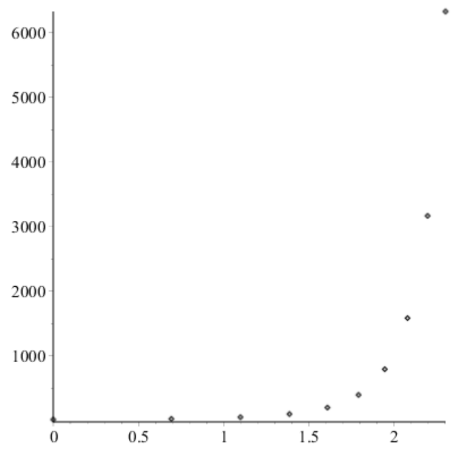

Figure 10: A plot of the growth of the heights of the iterates of x for the map in (142).

into why the presence of a transcendental integral causes the lack of integrability of the map when using the Hirota-Kimura discretization scheme.

Chapter 5

Hamiltonian systems with two degrees of freedom

In this chapter the Hénon-Heiles system will be used as an example of a Hamiltonian system with two degrees of freedom, and Kahan's discretization will be applied to a particular integrable case and then compared to the Bäcklund transformation. The Hénon-Heiles system was first introduced in 1964 to model the dynamics of a star within the galaxy. It is a two body system which describes motion in the plane using coordinates $\mathbf{q} = (q_1, q_2)$, the position vector of the particle and $\mathbf{p}(= \dot{\mathbf{q}}) = (p_1, p_2)$ the momentum vector. The potential can be constructed by the addition of two cubic terms to the potential of the planar harmonic oscillator to give

$$U(\mathbf{q}) = Aq_1^2 + Bq_2^2 + Cq_2^2 q_1 + Dq_1^3. \tag{144}$$

The kinetic energy of the particle can be written as $T(\mathbf{p}) = \frac{1}{2}(p_1^2 + p_2^2)$ and combining this with the potential shown above we have the Hamiltonian

$$H(q, p) = T(\mathbf{p}) + U(\mathbf{q}) = \frac{1}{2}(p_1^2 + p_2^2) + Aq_1^2 + Bq_2^2 + Cq_2^2 q_1 + Dq_1^3. \tag{145}$$

This Hamiltonian represents the total energy of the system which is conserved along all orbits. The equations of motion for this system are calculated using

$$\dot{\mathbf{q}} = \frac{\partial H(\mathbf{q},\mathbf{p})}{\partial \mathbf{p}}, \qquad \dot{\mathbf{p}} = -\frac{\partial H(\mathbf{q},\mathbf{p})}{\partial \mathbf{q}}, \tag{146}$$

to give

$$\dot{q_1} = p_1, \qquad \dot{q_2} = p_2, \tag{147}$$

$$\dot{p_1} = -Cq_2^2 - 2Aq_1 - 3Dq_1^2, \qquad \dot{p_2} = -2Bq_2 - 2Cq_1q_2. \tag{148}$$

5.1 The Integrable cases of the Hénon-Heiles system

The three integrable cases of the Hénon-Helies system are given in terms of the parameters (A, B, C, D) presented in the Hamiltonian (145) and are as follows:

Case (i): $A = B, D = \frac{1}{3}C$,

Case (ii): A, B arbitrary, $D = 2C$,

Case (iii): $B = 16A, D = \frac{16}{3}C$.

These cases can also be derived through the traveling wave reduction of fifth-order soliton equations. Case (i) is achieved by the reduction of the SK (Sawada-Kotera) equation [54], case (ii) by the reduction of the KdV5 equation [35] and case (iii) by the reduction of the KK (Kaup-Kupershmidt) equation [34, 14]. The derivation of case (ii) will be presented in the next section.

5.2 Derivation of case (ii) by the reduction of fifth order KdV equation

The fifth order KdV partial differential equation that will be reduced to give an example of a case (ii) Hénon-Heiles system of ODE's is given as

$$u_t = u_{xxxxx} + 10uu_{xxx} + 20u_x u_{xx} + 30u^2 u_x, \tag{149}$$

where u_t and u_x represent the partial derivatives of the function $u = u(x, t)$. This PDE can also be written as

$$u_t = (\mathrm{D}^3 + 4u\mathrm{D} + 2u_x)(u_{xx} + 3u^2), \tag{150}$$

to which we apply the travelling wave reduction of $w = u(z)$, $z = x - ct$ to give

$$(\mathrm{D}^3 + 4w\mathrm{D} + 2w')(w'' + 3w^2 + \frac{c}{2}) = 0, \qquad f = w'' + 3w^2 + \frac{c}{2}. \tag{151}$$

Expanding this gives the following ODE in f

$$ff'' - \frac{1}{2}(f')^2 + 2wf^2 + \frac{l^2}{2} = 0 \tag{152}$$

with $\frac{l^2}{2}$ being a constant of integration. If we take $f = -\frac{1}{2}q_2^2$ and $w = q_1$ then we arrive at the following system of ODE's

$$q_1'' + 3q_1^2 + \frac{c}{2} + \frac{1}{2}q_2^2 = 0, \qquad q_2'' + q_1 q_2 + \frac{l^2}{q_2^3} = 0. \tag{153}$$

With $p_1 = q_1'$ and $p_2 = q_2'$ we have a Hénon-Heiles system with Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) + q_1^3 + \frac{1}{2}q_1 q_2^2 - \frac{l^2}{2q_2^3} + \frac{c}{2}q_1. \tag{154}$$

If we consider the case with $l = 0$ then we can write down the steady states of this system in terms of c. The four fixed points and their stability for the variables (p_1, p_2, q_1, q_2) are

$$
\begin{aligned}
(0, 0, \mu, 0) &:\text{elliptic (center)} \\
(0, 0, -\mu, 0) &:\text{hyperbolic (saddle)} \\
(0, 0, 0, \sqrt{6}\mu) &:\text{hyperbolic (saddle-ellipse)} \\
(0, 0, 0, -\sqrt{6}\mu) &:\text{hyperbolic (saddle-ellipse)}
\end{aligned}
$$

with $c = -6\mu^2$.

The next sections will focus on this example with $c = -6$ to give real steady states.

5.3 Kahan's method

Here we will apply Kahan's method the following particular example of a case (ii) Hénon-Heiles system:

$$\dot{q_1} = p_1, \qquad \dot{q_2} = p_2, \tag{155}$$

$$\dot{p_1} = -\frac{1}{2}q_2^2 - 3q_1^2 + 3, \qquad \dot{p_2} = -q_1 q_2, \tag{156}$$

which has four real steady states $(0, 0, \pm 1, 0)$ and $(0, 0, 0, \pm\sqrt{6})$. The map created using Kahan's method takes the form

$$\frac{\tilde{q_1} - q_1}{h} = \frac{\tilde{p_1} + p_1}{2}, \qquad \frac{\tilde{q_2} - q_2}{h} = \frac{\tilde{p_2} + p_2}{2}, \tag{157}$$

$$\frac{\tilde{p_1} - p_1}{h} = -\frac{1}{2}q_2\tilde{q_2} - 3q_1\tilde{q_1} + 3, \qquad \frac{\tilde{p_2} - p_2}{h} = -\frac{q_1\tilde{q_2} + \tilde{q_1}q_2}{2}. \tag{158}$$

If we take initial conditions close to the elliptic fixed point $(0, 0, 1, 0)$ then we expect to see a closed compact orbit if this map is to preserve the qualitative features of the continuous system. The following plots have been created using the intial conditions $(0.1, 0.1 - 1.1, 0.1)$ and stepsize $h = 0.01$ and $n = 10000$. Figures 11, 12, 13 show clearly that the stability of the elliptic fixed point is indeed the same for the discrete system as it is for the continuous system.

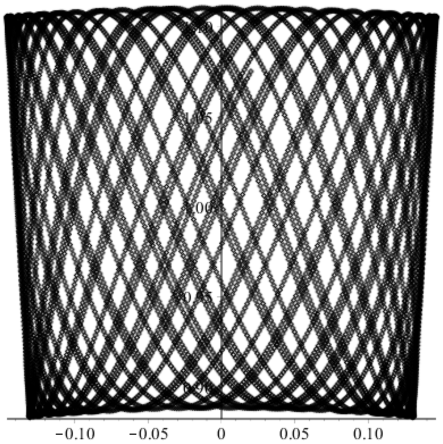

Figure 11: The iteration plot of q_1 and q_2 with initial conditions $(0.1, 0.1, -1.1, 0.1)$.

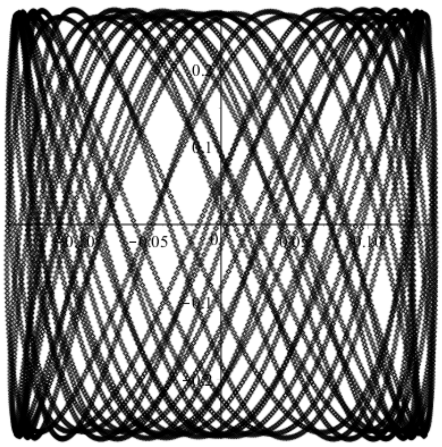

Figure 12: The iteration plot of p_1 and p_2 with initial conditions $(0.1, 0.1, -1.1, 0.1)$.

We can also check whether the Hamiltonian $H = \frac{1}{2}(p_1^2 + p_2^2) + q_1^3 + \frac{1}{2}q_1 q_2^2 - 3q_1$ is preserved under the time-step by plotting the value of H against n. As figure

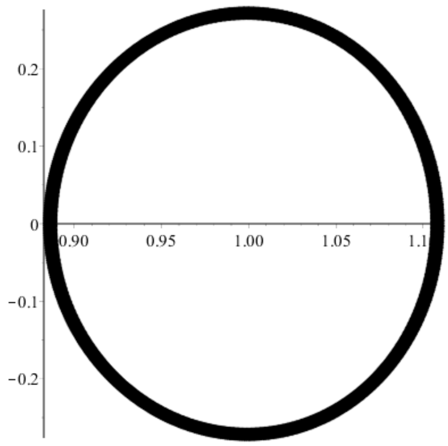

Figure 13: The iteration plot of p_1 and q_1 with initial conditions $(0.1, 0.1, -1.1, 0.1)$.

14 shows the map does not exactly preserve the value of H, but it does stay in the neighbourhood of -1.95 to three significant figures.

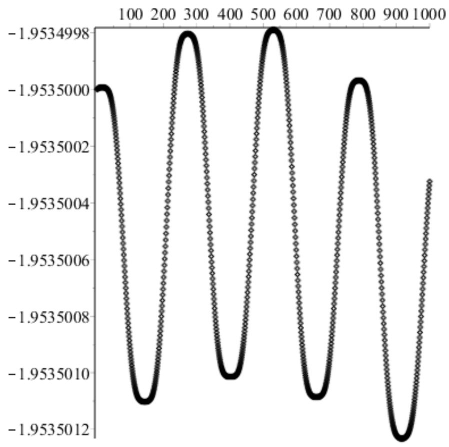

Figure 14: The value of H against n for 1000 iterations with initial conditions $(0.1, 0.1, -1.1, 0.1)$.

5.4 Diophantine integrability test on Kahan's method

To give an indication of the integrability of Kahan's method for this case (ii) Hénon-Heiles system we will now check whether the discrete system is Diophantine integrable. Figure 15 shows the logarithm of the heights of the first 10 q_1 iterates, and it is clear that the growth of the heights is greater than that of a polynomial. Therefore we can say that the discrete system (157),(158) is not Diophantine integrable.

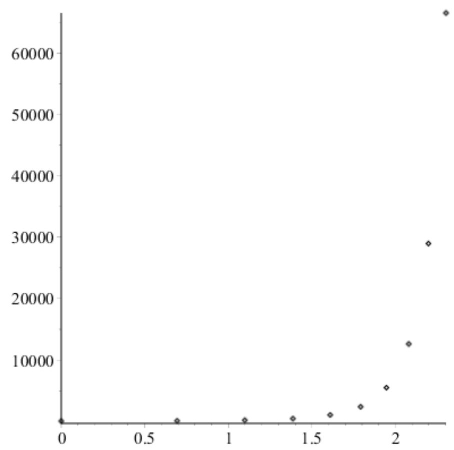

Figure 15: A plot of the growth of the logarithm of the heights of the iterates of q_1.

5.5 The Bäcklund transformation

As a comparison to Kahan's method we will now consider the Bäcklund transformation of a particular example of case (ii). The Bäcklund transformation for the many-body generalization of case (ii) is given in [25] which we will use to present our particular example (the original case - parameter values $c = m_j = a_j = 0$ and $n = 1$ in [25]).

First we need to give the Lax matrix L for this system:

$$L(\lambda) = \begin{pmatrix} \frac{p_1 q_1}{\lambda} & -\frac{p_1^2}{\lambda} \\ \frac{q_1^2}{\lambda} & -\frac{p_1 q_1}{\lambda} \end{pmatrix} + B(\lambda), \tag{159}$$

where the matrix $B(\lambda)$ is given as

$$B(\lambda) = \begin{pmatrix} -4p_2 & E \\ -16\lambda - 8p_2 & 4p_2 \end{pmatrix}, \qquad E = -16\lambda^2 + 8\lambda q_2 - 4q_2^2 - q_1^2. \tag{160}$$

The equations for the Bäcklund transformation are found from the entries of the matrix created by the discrete Lax equation

$$\tilde{L}M - ML = 0, \tag{161}$$

where $\tilde{L}$ is the updated Lax matrix with the variables replaced with their images under the Bäcklund transformation, and M is the Darboux matrix

$$M = \begin{pmatrix} -y & 1 \\ y^2 + \alpha - \lambda & -y \end{pmatrix}, \qquad y = -\sqrt{\lambda - \frac{1}{2}(q_2 + \tilde{q}_2)}. \tag{162}$$

The entires of the discrete Lax equation matrix are polynomials in λ and the equations for the Bäcklund transformation are found by requiring the coefficients of λ to be zero.

5.6 Conclusion

In this Chapter we have applied the Hirota-Kimura/Kahan discretization scheme to an example of the integrable case (ii) Hénon-Heiles system and showed that although the fixed points of the continuous system and their stability are preserved in the discrete system, the Hamiltonian is not. Also we apply the Diophantine integrability test to the map and discover that it is not integrable, unlike the continuous system. As a comparison to the map produced by the Hirota-Kimura/Kahan type discretization we have also mentioned the Bäcklund transformation for the same Hénon-Heiles system, which is exact in the sense that it preseves the Hamiltonians and it is symplectic. Although it is clear that the Bäcklund transformation produces a map with favourable features, Kahan's method as it is much simpler, explicit and will likely give similar results for all of the Hénon-Heiles systems, whereas the Bäcklund transformations for each case are quite complicated.

This work could be extended by applying Kahan's method to other examples of the integrable cases of the Hénon-Heiles system and look for any outcomes where it does produce a map that preserves the Hamiltonian.

Chapter 6

Systems with cubic vector fields and Limit Cycles

6.1 General Non-Standard Discretizations of a Trimolecular System

In this chapter we will be looking at a cubic system of first order differential equations which arise from a trimolecular reaction. This system is of particular interest as it has a solution which includes a limit cycle and we seek to produce one or more discrete models of the system which also have a limit cycle in their solution. A limit cycle is an isolated solution of the system which is periodic and corresponds to a closed curve in the phase space. This system is a result of applying the Law of Mass Action to the following reaction scheme:

$$X \to A, \qquad B \to Y, \qquad 2X + Y \to 3X. \tag{163}$$

In this reaction scheme A, B, X, Y are four molecular species and $k_j, j = 1, 2, 3, 4$ are the rate constants. If we assume the concentrations of A and B are kept constant (denoted a, b respectively), and we non-dimensionalise the resulting system from applying the Law of Mass Action then we have the following:

$$\dot{x} = a - x + x^2 y, \qquad \dot{y} = b - x^2 y \tag{164}$$

where x, y are the scaled concentrations of X, Y respectively. This system has a fixed point at $(x^*, y^*) = (a+b, b/(a+b)^2)$ which lies inside the limit cycle that is produced in the parameter range $b - a > (a+b)^3$ with $0 \leqslant b < 1$ (see chapter 7 in [22] for details). The system has a pair of complex conjugate eigenvalues which cause a stable spiral for $b - a < (a+b)^3$ and then a Hopf Bifurcation occurs along the line $b - a = (a+b)^3$ where the spiral becomes unstable, and a limit cycle is formed. We can derive the equation of the curve $b - a = (a+b)^3$ in the parameter space (a, b) by looking at the Jacobian of the system evaluated at the fixed point, and performing stability analysis. This gives us the Jacobian:

$$J|_{(x*,y*)} = \begin{pmatrix} -1 + \frac{2b}{(a+b)} & (a+b)^2 \\ \frac{-2b}{(a+b)} & -(a+b)^2 \end{pmatrix} \tag{165}$$

From this we have the determinant $D = (a+b)^2$ and the trace $T = \frac{2b}{(a+b)} - 1 - (a+b)^2 = \frac{2b-a-b-(a+b)^3}{a+b} = \frac{b-a-(a+b)^3}{a+b}$. Clearly $D > 0$ as $a > 0, b > 0$ and for the trace we have an equation which determines whether $T > 0$ or $T < 0$ which gives either an unstable spiral or a stable spiral respectively. Therefore we have a stable spiral for $b - a < (a+b)^3$, and then a Hopf bifurcation at $b - a = (a+b)^3$ and an unstable spiral and a limit cycle appear for $b - a > (a+b)^3$.

In an article by Hone [26] this exact system was discretized using ideas from Micken's approach [40] with seven parameters, all of which were constrained to take just one possible value in order for the system to be bi-rational, giving just one possible system with an inverse. However, this has been extended this slightly by introducing the maximum number of possible parameters into the discrete scheme which totals to eleven. This has been done in the hope that additional possibilities for the values of the parameters will be discovered and therefore one or more new discrete system will be uncovered.

6.1.1 The general non-standard discretization

The set up for this discretization is to take a system of differential equations:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$$

and replace the differential term with the usual forward step

$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\epsilon},$$

where ϵ is the step size and $\mathbf{x}_n$ is the value at step n. The right hand side, $\mathbf{f}(\mathbf{x})$ is then replaced with a new function $\mathbf{F}(\mathbf{x}_n, \mathbf{x}_{n+1})$ which will be an estimation of the original function.

In the system (164) we have linear and cubic terms which need to be dealt with for the discretization. One of the ideas for the Mickens approach is to take a kind of average of all the possible combinations of each term using the variables and their up-shifted value. For example, when discretizing a quadratic term xy there are four ways of combining the variables: $(xy, \tilde{x}y, x\tilde{y}, \tilde{x}\tilde{y})$ where x and $\tilde{x}$ represent x_n and x_{n+1} respectively. This form of discretization gives the following result on (164):

$$\frac{\tilde{x} - x}{\epsilon} = a - cx - (1-c)\tilde{x} + dx^2y + ex\tilde{x}y + fx^2\tilde{y} + g\tilde{x}^2y + hx\tilde{x}\tilde{y} + (1-d-e-f-g-h)\tilde{x}^2\tilde{y}, \tag{166}$$

$$\frac{\tilde{y} - y}{\epsilon} = b - Dx^2y - Ex\tilde{x}y - Fx^2\tilde{y} - G\tilde{x}^2\tilde{y} - Hx\tilde{x}y - (1-D-E-F-G-H)\tilde{x}^2\tilde{y}. \tag{167}$$

where (a, b) are constants and $(c, d, e, f, g, h, D, E, F, G, H)$ are the eleven parameters which we will be finding constraints for. The reason for this type of general average is so that as $\tilde{x}$ tends to x this discrete system tends to the original system, and therefore we will always get the same fixed points from the discrete system as we do in the original, which is of course one of the main features of the continuous system that we want to preserve.

In order to refine this discrete system so that it mimics the original system as closely as possible we now need to find conditions on the parameters which cause the system to be explicit for both the (x, y) and $(\tilde{x}, \tilde{y})$ variables which will give us a birational system. We will then be able to write (166) and (167) as the following:

$$(166) : \tilde{x} = f_1(x, y), \qquad \text{or} \qquad x = \tilde{f}_1(\tilde{x}, \tilde{y}), \tag{168}$$

$$(167) : \tilde{y} = f_2(x, y), \qquad \text{or} \qquad y = \tilde{f}_2(\tilde{x}, \tilde{y}). \tag{169}$$

where $f_i, \tilde{f}_i$, $i = 1, 2$ are rational functions yet to be determined.

6.1.2 Finding the Parameter Constraints

To achieve these constraints in the most efficient way we will use resultants as defined in Appendix A. Resultants are particularly useful for generating constraints on the parameters by requiring the function $R_{P,Q}$ have just one solution for the corresponding variable. For example if we compute the resultant for $\tilde{x}$ then we're left with a polynomial in x, and if coefficients are eliminated so that $R_{P,Q}(\tilde{x}) = 0$ has one solution then the solution we have will in fact be the function $\tilde{f}_1(\tilde{x}, \tilde{y})$ as described in (168), and similarly for the other variables. For our calculation the two functions P, Q will be as follows:

$$P = a-cx-(1-c)\tilde{x}+dx^2y+ex\tilde{x}y+fx^2\tilde{y}+g\tilde{x}^2\tilde{y}+hx\tilde{x}\tilde{y}+(1-d-e-f-g-h)\tilde{x}^2\tilde{y}-\frac{(\tilde{x}-x)}{\epsilon}, \tag{170}$$

$$Q = b-Dx^2y-Ex\tilde{x}y-Fx^2\tilde{y}-G\tilde{x}^2\tilde{y}-Hx\tilde{x}\tilde{y}-(1-D-E-F-G-H)\tilde{x}^2\tilde{y}-\frac{(\tilde{y}-y)}{\epsilon}. \tag{171}$$

Then we have four resultants to use for the constraints as we can look at P, Q as polynomials in either $\tilde{x}, \tilde{y}, x$ or y variables, and treat the remaining variables as constants. However the resultants are paired as each variable and its unshifted counterpart to have their resultants satisfied simultaneously so a bi-rational system is produced. So we need to find constraints on the parameters which give one solution for both $R_{P,Q}(\tilde{x}) = 0$ and $R_{P,Q}(x) = 0$ and then also for both $R_{P,Q}(\tilde{y}) = 0$ and $R_{P,Q}(y) = 0$.

When the resultant is performed on one of these functions a new function is formed which will be treated as a polynomial in the other variable, so if the resultant was computed with $\tilde{x}$ as the variable, then the new function formed would be considered to be a polynomial in $\tilde{y}$, and the same for x, y and the inverses. This new function will always be a polynomial of degree 4, however as only one solution should be produced when set to zero certain coefficients need to be eliminated. Consider this new function in the form

$$p_4x^4 + p_3x^3 + p_2x^2 + p_1x + p_0 = 0, \tag{172}$$

where $p_i,\ i = 0, .., 4$ are the coefficients and x represents one of the variables $\tilde{x}, \tilde{y}, x, y$. The obvious choice of coefficients to eliminate are p_4, p_3 and p_2 so that we are left with $p_1x+p_0 = 0$ which gives the desired single solution $x = \frac{-p_0}{p_1}$. However there also other choices which give equations with a single solution provided we assume $x = 0$ cannot be a solution. These are outlined below:

$$p_4 = p_3 = p_2 = 0 \quad \Rightarrow \quad p_1 x + p_0 = 0 \quad \Rightarrow x = \frac{-p_0}{p_1}, \tag{173}$$

$$p_4 = p_3 = p_0 = 0 \quad \Rightarrow \quad x(p_2 x + p_1) = 0 \quad \Rightarrow x = \frac{-p_1}{p_2}, \tag{174}$$

$$p_4 = p_1 = p_0 = 0 \quad \Rightarrow \quad x^2(p_3 x + p_2) = 0 \quad \Rightarrow x = \frac{-p_2}{p_3}, \tag{175}$$

$$p_2 = p_1 = p_0 = 0 \quad \Rightarrow \quad x^3(p_4 x + p_3) = 0 \quad \Rightarrow x = \frac{-p_3}{p_4}. \tag{176}$$

These conditions will be what we will use as constraints as each p_i will be a function of the variables and the parameters so setting the parameters to take certain values will lead to the coefficient vanishing. It is possible that we may come across situations where even after eliminating all the parameters in a coefficient we may be left with either variables with constant coefficients or an expression in ϵ, neither of which can be set to zero, and therefore we cannot retrieve a constraint from that particular condition.

6.1.3 Resultants for $\tilde{x}$ and x.

Note: *Most of the equations for the parameters found in these next two sections are the most simplified versions of the coefficients $\{p_i\}$ with all the common factors having been removed.*

The first resultant computed is the one for $\tilde{x}$ which as stated above gives a polynomial in $\tilde{y}$ of degree 4. Condition (173) from above is the first to be considered and initially we have to eliminate p_4 which in this case is itself a polynomial in x of degree 4. Most of the coefficients in the resultant for $\tilde{x}$ are significantly more complex than those for $\tilde{y}$ and therefore will not be displayed in this section, however the coefficients for $\tilde{y}$ are compact enough to be quoted in the following section. Inspecting p_4 we discover that the most general option for the elimination of this coefficient is a choice of parameter values such that

$D + E + F + G + H = 1, \quad d + e + f + g + h = 1.$

Next we look at p_3, and as we want this to vanish simultaneously with p_4 we can substitute the parameter values we just found straight into p_3. Having substituted $H = 1 - D - E - F - G$ and $h = 1 - d - e - f - g$ into p_3 we find that the only extra condition needed to cause it to vanish is $G = g = 0$. Conveniently we also discover that these parameter values eliminate p_2, p_1 and p_0 and therefore make the whole resultant vanish. This is seen as a null result as it does not give any solution, and as a result there is no point investigating the resultant with respect to x as we need both resultants to have a unique solution to give a birrational system.

6.1.4 Resultants for $\tilde{y}$ and y.

Firstly we will look at (173), which means eliminating p_4, p_3 and p_2. The constraint $p_4 = 0$ applied to the resultant with respect to $\tilde{y}$, which in this case is the coefficient of $\tilde{x}^4$, gives the following equation:

$$p_4 = G(1 - d - e - f - h) - g(1 - D - E - F - H) = 0. \tag{177}$$

This coefficient is only in terms of the parameters and it is therefore easy to see values of these parameters which will cause p_4 to vanish. There are three ways to achieve this, firstly we can take $G = g = 0$, and secondly we could take $d+e+f+h = 1$ and $D+E+F+H = 1$ and thirdly we could take $g = 1-d-e-f-h$ and $G = 1 - D - E - F - H$. If we take $G = g = 0$ first and apply this to p_3, which in this case is a monmial in x, we have the following two parts of p_3 which both need to be eliminated:

$$\text{Coeff of } x \text{ in} \quad p_3 := E(1 - d - f - h) + e(1 - D - F - H), \tag{178}$$

From (178) we can see that taking $E = e = 0$ will eliminate the coefficient of x, but it will not do the same for the constant term so this is not useful. However, taking $E = 0$ along with $D + F + H = 1$ does in fact eliminate both parts giving $p_3 = 0$. Now we just need to ensure $p_2 = 0$ is satisfied and we have found one set of parameter values which give the condition (173) and causes the resultant with respect to $\tilde{y}$ to have only one solution. Using the constraints $G = g = 0$, $E = 0$ and $H = 1 - D - F$ substituted into p_2 we have the following parts which all need to be eliminated:

$$\text{Coeff of } x^2 \text{ in} \quad p_2 := (1 - d - f - h)D + (1 - F)e, \tag{179}$$

$$\text{Coeff of } x \text{ in} \quad p_2 := \{(1 - D - F)c + F + D - 1\}\epsilon + F + D - 1, \tag{180}$$

$$\text{Coeff of } x^0 \text{ in} \quad p_2 := (1 - d - e - f - h)b\epsilon + (1 - d - e - f - h)y. \tag{181}$$

Straight away we can see that the only option for the elimination of the constant term is $d + e + f + h = 1$, and similarly there is only one option for the elimination of the coefficient of x, namely $D + F = 1$. Taking $h = 1 - d - e - f$ and $F = 1 - D$ we conveniently find that the coefficient of x^2 also vanishes. The condition $F = 1 - D$ results in $H = 0$ as $H = 1 - D - F$ from before. So this gives us our first provisional set of parameter values for the resultant with respect to $\tilde{y}$ which are:

$$\text{Provisional Set 1}: E = 0, \quad G = g = 0, \quad H = 0, \quad h = 1 - d - e - f, \quad F = 1 - D \tag{182}$$

Now we return to p_4 as we had two other options which caused p_4 to vanish, and now we will assess the second option, which was $d + e + f + h = 1$ and $D + E + F + H = 1$. So if we subsitute $h = 1 - d - e - f$ and $H = 1 - D - E - F$ into p_3 we have the following:

$$\text{Coeff of } x \text{ in} \quad p_3 := (1-D-F)g + (1-d-f)G, \tag{183}$$

$$\text{Coeff of } x^0 \text{ in} \quad p_3 := G(1+\epsilon - c\epsilon). \tag{184}$$

Clearly we need $G = 0$ to eliminate the constant term here, and then we have two options again for the coefficient of x, which are $g = 0$ or $D + F = 1$. Dealing with $g = 0$ first and substituting this into p_2 we have:

$$\text{Coeff of } x^2 \text{ in} \quad p_2 := (1-D-F)e - (1-d-f)E, \tag{185}$$

$$\text{Coeff of } x \text{ in} \quad p_2 := \{(1-D-E-F)c-(1-D-E-F)\}\epsilon-(1-D-E-F). \tag{186}$$

The coefficient of x gives no choice but $D + E + F = 1$. Substituting $F = 1 - D - E$ into (185) gives $E(1 - d - e - f)$. Once again we have two choices: $E = 0$ or $d + e + f = 1$. So for the option $g = 0$ from p_4 we have two more provisional sets of parameter values:

$$\text{Provisional Set 2}: E = 0, \quad G = g = 0, \quad H = 0, \quad h = 1-d-e-f, \quad F = 1-D, \tag{187}$$

$$\text{Provisional Set 3}: G = g = 0, \quad H = h = 0, \quad f = 1-d-e, \quad F = 1-D-E. \tag{188}$$

Straight away it is clear that provisional set 2 (187) is identical to provisional set 1(182) so in fact we only have two sets of parameter values.

Now we go back to the other option, namely $D + F = 1$, and we substitute $F = 1 - D$ and $H = E$ into p_2 to give:

$$\text{Coeff of } x^2 \text{ in} \quad p_2 := (2e+f-1-d)E + g, \tag{189}$$

$$\text{Coeff of } x \text{ in} \quad p_2 := (3c-1)E\epsilon - 3E. \tag{190}$$

Here the coefficient of x gives $E = 0$ as only option, and this substituted into (189) gives $g = 0$. Now we have a fourth provisional set of parameter values:

$$\text{Provisional Set 4}: E = 0, \quad G = g = 0, \quad H = 0, \quad h = 1-d-e-f, \quad F = 1-D. \tag{191}$$

Again we have a copy of the first provisional set (182), so we can conclude that we still only have two sets of parameter values so far, which are outlined below:

$$\text{Set 1}: E = 0, \quad G = g = 0, \quad H = 0, \quad h = 1 - d - e - f, \quad F = 1 - D, \tag{192}$$

$$\text{Set 2}: G = g = 0, \quad H = h = 0, \quad f = 1 - d - e, \quad F = 1 - D - E. \tag{193}$$

Finally we shall now look at the third option for the parameters which eliminate p_4, which were $g = 1 - d - e - f - h$ and $G = 1 - D - E - F - H$. Substituting this into p_3 gives the following:

$$\text{Coeff of } x \text{ in} \quad p_3 := (1 - d - e - f)H - (1 - D - E - F)h, \tag{194}$$

Eliminating the coefficient here requires one of three options for the parameters: (1) $H = h = 0$, (2) $d + e + f = 1$ and $D + E + F = 1$, (3) $h = 1 - d - e - f$ and $H = 1 - D - E - F$. Substituting $H = h = 0$ into p_2 gives the following:

$$\text{Coeff of } x^2 \text{ in} \quad p_2 := (1 - d - e)F - (1 - D - E)f, \tag{195}$$

$$\text{Coeff of } x^0 \text{ in} \quad p_2 := 1 - d - e - f. \tag{196}$$

Again there are a few choices here, firstly we could take $F = 0$ and $f = 0$ which results in needing $d + e = 1$ and therefore $g = 0$ and $G = 1 - D - E$. Secondly we could take $f = 1 - d - e$ and $F = 1 - D - E$ which also results in $G = g = 0$.

Now substituting the second choice (2) $d + e + f = 1$ and $D + E + F = 1$, which also gives $G = H$ and $g = h$, into p_2 we have:

$$\text{Coeff of } x^2 \text{ in } \quad p_2 := (2e - d - 1)H - (2E - D - 1)h, \tag{197}$$

$$\text{Coeff of } x \text{ in } \quad p_2 := (3c\epsilon - \epsilon - 3)H, \tag{198}$$

$$\text{Coeff of } x^0 \text{ in } \quad p_2 := (y + 2b\epsilon)h + 2a\epsilon H. \tag{199}$$

The only choice here is $H = h = 0$, however we can discard this result as it is identical to the one discovered previously. The third option was (3) $h = 1 - d - e - f$, $H = 1 - D - E - F$ and therefore $G = g = 0$. These values substituted into p_2 gives the following constraints:

$$\text{Coeff of } x^2 \text{ in } \quad p_2 := (1 - D - F)e - (1 - d - f)E, \tag{200}$$

$$\text{Coeff of } x \text{ in } \quad p_2 := \{(1-D-E-F)c-(1-D-E-F)\}\epsilon-(1-D-E-F). \tag{201}$$

Here we have two options, either $E = 1-D-F$ and $e = 1-d-f$, or $E = e = 0$ and $F = 1 - D, \quad f = 1 - d$. The first option is again identical to a previous result, and the second option is just a particular case of that result.

The next step is to look at the other coefficient constraints, (174), (175) and (176). However, it is not actually possible to do these as we cannot use parameter values to eliminate the coefficients p_1 and p_0. For p_1 we find the constant term $c\epsilon - \epsilon - 1$ which cannot be eliminated as setting $c = \frac{1+\epsilon}{\epsilon}$ will alter the behaviour of the system. Similarly for p_0 we have the constant term $a\epsilon$ and also the coefficient of x: $1 - c\epsilon$, neither of which can be eliminated for the same reason.

These sets of parameter values, (192) and (193), will allow us to write the original system in the form $\tilde{x} = f_1(x, y)$ and $\tilde{y} = f_2(x, y)$, but we also need to be able write the system inversely, so now we need to find additional constraints on the parameters by looking at the resultant with respect to y. As we need both resultants to be satisfied simultaneously we can use the parameter sets (192) and (193) to simplify the resultant of y. As we did with the resultant for $\tilde{y}$ we find that we cannot use the coefficient constraints (174), (175) and (176) due to terms which cannot be eliminated, which are as follows:

$$\text{Coeff of } \tilde{x}^0 \text{ in } \quad p_0 := a\epsilon, \tag{202}$$

$$\text{Coeff of } \tilde{x} \text{ in } \quad p_0 := 1 + \epsilon - c\epsilon, \tag{203}$$

$$\text{Coeff of } \tilde{x}^0 \text{ in } \quad p_1 := c\epsilon - 1. \tag{204}$$

So this leaves us with only (173) to use to find extra constraints. Starting with p_4 and substituting the parameter values from set 1 we have the following:

$$(f + d)D - d, \tag{205}$$

which gives the only option of $D = 0$ and $d = 0$. Substituting these into p_3 gives $e = 0$, and then for p_2 we get $f = 0$. Now we have a complete set of parameter values for set 1 which will give a birational system.

Now we look at the parameter values from set 2 for the resultant with respect to y. Here we encounter a problem in that p_2 with these particular parameter values cannot be eliminated. If we look at p_2 we can see why:

$$p_2 : \quad (c\epsilon\tilde{x} - \epsilon\tilde{x} - \tilde{x} + a\epsilon)D + (\tilde{x} - c\epsilon\tilde{x})E + b\epsilon d + \tilde{y}e - \tilde{y}, \tag{206}$$

Even with taking $D = 0, E = 0, d = 0, e = 0$ we are still left with the term $-\tilde{y}$ and so we can now discard parameter set 2 as we cannot use the parameter values in it to make the system birational.

Finally we need to assess the resultant for y using the parameter values in set 3. These values conveniently eliminate p_4, so we just need to look at p_3 and p_2, which are shown below:

$$p_3: \quad (1 - c\epsilon)D, \tag{207}$$

$$p_2: \quad (c\epsilon\tilde{x} - \epsilon\tilde{x} - \tilde{x} + a\epsilon)D + (\tilde{x} - c\epsilon\tilde{x})E - (b\epsilon - \tilde{y})d. \tag{208}$$

From this we find the parameter values $D = 0, E = 0, d = 0$ cause both p_2 and p_3 to vanish, and as a result we have the second and last set of parameter values which give a birational system. These two parameter sets are outlined below:

$$\text{Final Set 1}: \quad d = 0, e = 0, f = 0, g = 0, h = 1, \qquad D = 0, E = 0, F = 1, G = 0, H = 0. \tag{209}$$

$$\text{Final Set 2}: \quad d = 0, e = 1, f = 0, g = 0, h = 0, \qquad D = 0, E = 0, F = 0, G = 1, H = 0. \tag{210}$$

As has been found in other discrete systems, such as the Lotka-Volterra system, we find that the parameter for the linear part of the system, in this case c, is left with no constraint and can take any value.

6.2 The Final Result

Now that we have the only feasible parameter values that give a birational system we are finished with investigating the resultants from the most general version of the discrete system. We now have the following two maps, both of which only have the parameter c left from the new parameters introduced in (166) and (167):

$$\frac{\tilde{x} - x}{\epsilon} = a - cx - (1 - c)\tilde{x} + x\tilde{x}\tilde{y}, \qquad \frac{\tilde{y} - y}{\epsilon} = b - x^2\tilde{y}. \tag{211}$$

$$\frac{\tilde{x} - x}{\epsilon} = a - cx - (1 - c)\tilde{x} + x\tilde{x}y, \qquad \frac{\tilde{y} - y}{\epsilon} = b - \tilde{x}^2\tilde{y}. \tag{212}$$

Unfortunately we have not found any new ways to discretize this system beyond those found in [26] despite introducing a full range of parameters. Nonetheless this now confirms that these two are definitely the only possibilities for a bi-rational discretization of (164) using Micken's approach. In fact we only really have one discretization here as they are the inverses of each other.

Having found the only possibility for a bi-rational discrete system which is based on the original trimolecular system we can now investigate the existence of the limit cycle for certain values of the parameters a, b. To begin with we can check that we get a stable spiral for $b - a < (a + b)^3$ as we do in the original system, which as the plot below shows we do at least for one set of values that satisfy this inequality. In figure 16 we have $\epsilon = 0.05$ and $c = \frac{1}{2}$.

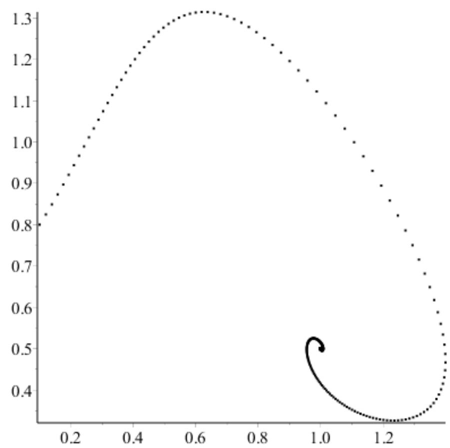

Figure 16: The iteration plot of the discrete system (211) with initial conditions $x_0 = 0.1, y_0 = 0.8$ and parameter values $a = b = \frac{1}{2}$.

Here we see that the iteration quickly spirals into the fixed point which in this case is $(a + b, \frac{b}{(a+b)^2}) = (1, \frac{1}{2})$ and therefore is behaving how we had hoped. Next we need to check to see if we get a limit cycle for parameters values defined by $b - a > (a + b)^3$. Figure 17 is with initial values which lie outside the limit cycle and so we see the plot spirals around into the limit cycle and stays there. The length of the iteration is 10000 steps but the plot hits the limit cycle after about 1500 steps. Again we have $\epsilon = 0.05$ and $c = \frac{1}{2}$.

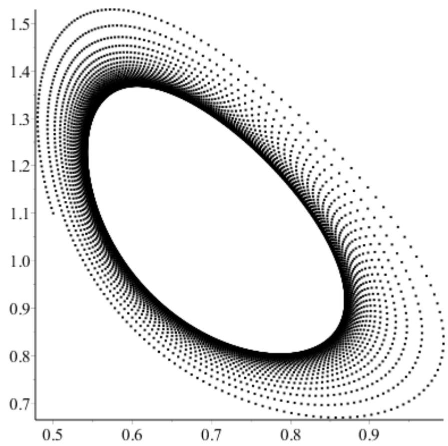

Figure 17: The iteration plot of the discrete system (211) with initial conditions $x_0 = 0.5, y_0 = 1.1$ and parameter values $a = \frac{9}{50}, b = \frac{1}{2}$.

We can also look at having the initial values being on the inside of the limit cycle and therefore the plot spiraling out to meet it.

So we have clear evidence that limit cycles do exist for certain values of the parameters in this discrete system, and for the above examples at least the parameter boundaries for the bifurcation appear to line up with the original system, however it is unlikely that the bifurcation line $b - a = (a + b)^3$ from the original system will hold for the discrete system due to the introduction of ϵ.

6.3 General Non-Standard Discretizations of a Hamiltonian System with a Quartic Potential

We will look at a Hamiltonian system with a quartic potential which gives a cubic system of Hamilton's equations.

$$H = \frac{1}{2}p^2 - \frac{a}{4}x^4 + \frac{b}{2}x^2 \tag{213}$$

$$\dot{x} = p, \qquad \dot{p} = ax^3 - bx. \tag{214}$$

We are using this particular Hamiltonian because it gives the possibility, (depending on the parameters a, b), of seeing a center at the fixed point $(0, 0)$ and therefore elliptic orbits around $(0, 0)$. The other two fixed points are $(\sqrt{\frac{b}{a}}, 0)$ and $(-\sqrt{\frac{b}{a}}, 0)$ which are both hyperbolic. Elliptic orbits in the original continuous system are preferable as they are a good visual structure to try to preserve in the discrete version of the system. Without such orbits numerical plots of the discrete system would be considerably less interesting.

The general form for this type of discretization is given below:

$$\frac{\tilde{x} - x}{h} = Ap + (1 - A)\tilde{p}, \tag{215}$$

$$\frac{\tilde{p} - p}{h} = a[Bx^3 + Cx^2\tilde{x} + Dx\tilde{x}^2 + (1 - B - C - D)\tilde{x}^3] - b[Ex + (1 - E)\tilde{x}]. \tag{216}$$

This gives us the 5 parameters A, B, C, D, E which will need to be constrained in order to give a bi-rational system, and then further constrained to give a symplectic system.

Again we will be using the resultant to ensure that the discrete system is birational, and fortunately this system requires little work as the constraint options within the resultant are limited.

6.3.1 Finding the constraints

First we need to define the functions that we will be applying the resultant to and set up some notation. The two functions will be labeled $P(x, p, \tilde{x}, \tilde{p})$ and $Q(x, p, \tilde{x}, \tilde{p})$ and appear as follows:

$$P = Ap + (1-A)\tilde{p} - \frac{\tilde{x}-x}{h}, \tag{217}$$

$$Q = a[Bx^3 + Cx^2\tilde{x} + Dx\tilde{x}^2 + (1-B-C-D)\tilde{x}^3] - b[Ex + (1-E)\tilde{x}] - \frac{\tilde{p}-p}{h}. \tag{218}$$

The resultant of P and Q will be expressed as $R_{\mathbf{x}}$ where $\mathbf{x} \in \{x, p, \tilde{x}, \tilde{p}\}$ where the lower index corresponds to the variable the functions P, Q are considered to be in. As the resultants with respect to a variable will give a polynomial in the opposite variable we have that $R_x = R_x(p), R_{\tilde{x}} = R_{\tilde{x}}(\tilde{p})$ and so on. These polynomials will all be of degree three and will therefore have the following structure:

$$R_{\mathbf{x}} = c_3\hat{\mathbf{x}}^3 + c_2\hat{\mathbf{x}}^2 + c_1\hat{\mathbf{x}} + c_0, \tag{219}$$

where $\hat{\mathbf{x}}$ is the 'opposite' variable to $\mathbf{x}$ and the coefficients c_i are themselves functions of the two remaining variables. Now we want to be able to solve this polynomial to give a unique solution so that we have a rational map. Achieving a bi-rational map then means ensuring there is also a unique solution from the resultant in the up shifted variable simultaneously. If we assume that we cannot have $\mathbf{x} = 0$ as a possibility we have three choices for setting the coefficients in (219) to zero to give a unique solution, which are as follows:

$$c_3 = c_2 = 0 \quad \Rightarrow \quad c_1\mathbf{x} + c_0 = 0 \quad \Rightarrow \mathbf{x} = \frac{-c_0}{c_1}, \tag{220}$$

$$c_3 = c_0 = 0 \quad \Rightarrow \quad c_2\mathbf{x} + c_1 = 0 \quad \Rightarrow \mathbf{x} = \frac{-c_1}{c_2}, \tag{221}$$

$$c_1 = c_0 = 0 \quad \Rightarrow \quad c_3\mathbf{x} + c_2 = 0 \quad \Rightarrow \mathbf{x} = \frac{-c_2}{c_3}, \tag{222}$$

6.4 Resultants for x and $\tilde{x}$.

Looking first at the resultant for x and applying the constraint $c_3 = c_2 = 0$ we have the following equations:

$$c_3 = 0 \quad \Rightarrow \quad -BA^3 = 0, \tag{223}$$

$$c_2 = 0 \quad \Rightarrow \quad (3B + C)A^2\tilde{x} + (A^3 - A^2)3hB\tilde{p} = 0. \tag{224}$$

It is clear that $A = 0$ will cause both coefficients to vanish, but there is also a second choice of $B = 0$ and $C = 0$ leaving A free.

Now applying the constraint $c_3 = c_0 = 0$ to the same resultant we know from above we need either $A = 0$ or $B = 0$ so we can substitute these straight into c_0 and look for further parameter constraints to cause it to vanish:

$$A = 0 \quad \Rightarrow \quad c_0 = ah\tilde{x}^3 - bh\tilde{x} + p = 0, \tag{225}$$

$$B = 0 \quad \Rightarrow \quad c_0 = ah\tilde{x}^3 + (ah^2AD - 2ah^2AC)p\tilde{x}^2 + (-bh + ah^3A^2Cp^2)\tilde{x} + (1 + bh^2AE)p = 0, \tag{226}$$

Here we can see that it is not possible to make c_0 vanish due to the terms p and $ah\tilde{x}^3$ that appear above, neither of which contain parameters which can be set to zero. In fact, these terms appear in c_0 before using the parameter constraints from $c_3 = 0$ and therefore it is also not possible to find any new parameter values by using the constraints $c_1 = c_0 = 0$. Having exhausted the choices for parameter values which give a unique solution of the resultant with respect to x we have two sets of parameter values which give a rational forward map. Now we can apply these values into $R_{\tilde{x}}$ (as both need to be solved simultaneously) and check for rationality in the backwards map.

Starting with the choice of $A = 0$ and looking at $c_3 = c_2 = 0$ we have the following parameter equations:

$$c_3 = 0 \quad \Rightarrow \quad B + C + D - 1 = 0, \tag{227}$$

$$c_2 = 0 \quad \Rightarrow \quad (3B + 3C + 2D - 3)x = 0, \tag{228}$$

Here (227) gives us that $D = 1 - B - C$ which substituted into (228) gives us $(B + C - 1)x = 0$ and therefore $D = 0, \quad C = 1 - B$. These two parameter constraints along with $A = 0$ is the first complete set which gives a bi-rational map. As we found with R_x $c_1 = c_0 = 0$ is also not possible for $R_{\tilde{x}}$ due to the presence of terms which cannot be eliminated using the parameters.

Now we need to check the case $B = 0, C = 0$ for $R_{\tilde{x}}$, which gives the following parameter equations:

$$c_3 = 0 \quad \Rightarrow \quad (1 - D)(A - 1)^3 = 0, \tag{229}$$

$$c_2 = 0 \quad \Rightarrow \quad 3hyA(D - 1)(A - 1)^2 + x(2D - 3)(A - 1)^2 = 0. \tag{230}$$

Here (229) gives two options of either $D = 1$ or $A = 1$. Using $D = 1$ in (230) only leads to needing $A = 1$ anyway, but using $A = 1$ first eliminates c_2 without the need for further parameter constraints. So here we have found a second set of parameter values which give a bi-rational map: $A = 1, B = 0, C = 0$. Now we have finished analysing the resultants for the x variables and have discovered two sets of parameter values, next we look at the resultants with respect to the p variables.

6.4.1 Resultants for p and $\tilde{p}$.

The calculations for R_p and $R_{\tilde{x}}$ are very similar to those done in the previous section. In fact they also lead to exactly the same outcome so we will not go through the calculation again, but instead state the two sets which come from them:

Parameter set 1): $A = 0$, $B = 1 - C$, $D = 0$ and C, E free.

Parameter set 2): $A = 1$, $B = 0$, $C = 0$ and D, E free.

6.5 The Bi-rational Maps

The two bi-rational discrete systems which emerged from the previous sections are as follows:

$$\frac{\tilde{x} - x}{h} = \tilde{p}, \qquad \frac{\tilde{p} - p}{h} = a[Bx^3 + (1 - B)x^2\tilde{x}] - b[Ex + (1 - E)\tilde{x}]. \tag{231}$$

$$\frac{\tilde{x} - x}{h} = p, \qquad \frac{\tilde{p} - p}{h} = a[Dx\tilde{x}^2 + (1 - D)\tilde{x}^3] - b[Ex + (1 - E)\tilde{x}]. \tag{232}$$

6.5.1 Finding the symplectic maps

Now we have found the only two possible discrete systems which are bi-rational, we can move on to confirming whether or not each is symplectic. The original system is symplectic with the canonical 2-form $\omega = dx \wedge dp$ and for the same 2-form to be preserved in a discrete version of this system we need the following:

$$d\tilde{x} \wedge d\tilde{p} = dx \wedge dp \qquad \Rightarrow \qquad \mathbf{Det}J = 1, \tag{233}$$

where J is the Jacobian of the system evaluated at any of the fixed points. If a system is symplectic then it can easily be shown that $\mathbf{det}J = 1$ for all fixed points, and therefore the product of the eigenvalues is always 1. This implies that each fixed point with eigenvalues λ_1, λ_2 must either be a saddle point, with $|\lambda_1| > 1$ and $|\lambda_2| < 1$ without loss of generality, or a center, with a complex conjugate pair of eigenvalues with $|\lambda_{1,2}| = 1$. For the discrete version of this particular system we need the fixed point $(0, 0)$ to be a center, and the other two $(\sqrt{\frac{b}{a}}, 0)$ and $(-\sqrt{\frac{b}{a}}, 0)$ to both be saddle points, which would give the correct qualitative imitation of the continuous system phase portrait.

We can check that our two discrete maps are symplectic or not by looking at the 2-form for each.We start with (231) and write the system in a simpler format:

$$\tilde{x} - x = h\tilde{p}, \qquad \tilde{p} - p = hf(\tilde{x}, x). \tag{234}$$

Now if we apply the exterior derivative we have the following:

$$d\tilde{x} - dx = d\tilde{p}, \tag{235}$$

$$d\tilde{p} - dp = f_{\tilde{x}} d\tilde{x} + f_x dx, \tag{236}$$

And then take the wedge product of $d\tilde{x}$ with (235) we have:

$$d\tilde{x} \wedge d\tilde{x} - dx \wedge d\tilde{x} = d\tilde{p} \wedge d\tilde{x} \qquad \Rightarrow \qquad -dx \wedge d\tilde{x} = d\tilde{p} \wedge d\tilde{x}, \tag{237}$$

and then doing the same but with dx:

$$d\tilde{x} \wedge dx - dx \wedge dx = d\tilde{p} \wedge dx \qquad \Rightarrow \qquad d\tilde{x} \wedge dx = d\tilde{p} \wedge dx. \tag{238}$$

Now seeing as $-dx \wedge d\tilde{x} = d\tilde{x} \wedge dx$ we have the following result:

$$d\tilde{p} \wedge dx = d\tilde{p} \wedge d\tilde{x} \tag{239}$$

We will use this soon, but now we need to look at the wedge product of (236) with dx:

$$d\tilde{p} \wedge dx - dp \wedge dx = f_{\tilde{x}} d\tilde{x} \wedge dx. \tag{240}$$

The $f_x dx$ term from (236) vanishes as $dx \wedge dx = 0$. Now we can use the results (239) and (237) to give the following:

$$d\tilde{p} \wedge d\tilde{x} - dp \wedge dx = f_{\tilde{x}} d\tilde{p} \wedge d\tilde{x}. \tag{241}$$

Reversing the order of the wedge products and rearranging we have

$$dx \wedge dp = (1 - f_{\tilde{x}}) d\tilde{x} \wedge d\tilde{p}, \tag{242}$$

and therefore we need $f_{\tilde{x}} = 0$ for (234) to be symplectic with the same symplectic structure as the original system.

A very similar calculation leads to almost the same result for the second system (243), also written in a simpler form:

$$\tilde{x} - x = hp, \qquad \tilde{p} - p = hg(\tilde{x}, x). \tag{243}$$

which give leads to the requirement that $g_x = 0$ as shown below:

$$dx \wedge dp = (1 - g_x) d\tilde{x} \wedge d\tilde{p}, \tag{244}$$

The next step is to calculate $f_{\tilde{x}}$ and g_x and evaluate at each of the fixed points and see if we can set parameters to certain values which will cause it to vanish.

$$f_{\tilde{x}} = a(1-B)x^2 - b(1-E), \tag{245}$$

$$g_x = aD\tilde{x}^2 - bE. \tag{246}$$

Analysing the above for the fixed point $x = \tilde{x} = 0$ we have the following:

$$f_{\tilde{x}}(0) = -b(1-E) = 0 \qquad \Rightarrow \qquad E = 1, \tag{247}$$

$$g_x(0) = -bE = 0 \qquad \Rightarrow \qquad E = 0. \tag{248}$$

The other two fixed points are $x = \tilde{x} = \sqrt{\frac{b}{a}}$ and $x = -\sqrt{\frac{b}{a}}$ but as both will give the same value when squared we just have the following:

$$f_{\tilde{x}}(\sqrt{\frac{b}{a}}) = b(1-B) = 0 \qquad \Rightarrow \qquad B = 1, \tag{249}$$

$$g_x(\sqrt{\frac{b}{a}}) = bD = 0 \qquad \Rightarrow \qquad D = 0, \tag{250}$$

So from these calculations we have two more constraints on the parameters for each map, and in fact all of the parameters are now fixed in order to make a symplectic birational map. These two discrete systems are displayed below:

$$\frac{\tilde{x}-x}{h} = \tilde{p}, \qquad \frac{\tilde{p}-p}{h} = ax^3 - bx. \tag{251}$$

$$\frac{\tilde{x}-x}{h} = p, \qquad \frac{\tilde{p}-p}{h} = a\tilde{x}^3 - b\tilde{x}. \tag{252}$$

In fact here we only see one map, as (252) is the inverse of (251) when $h \to -h$.

6.5.2 Integrability

Another quality we can investigate for this discrete system is whether or not it is integrable. Fortunately all of the possible integrable scalar difference equations which posses a non-trivial symmetric integral have been listed in chapter 20 of [55] so all we are required to do is compare this one to the list. In the book the difference equations have been written as a one dimensional two-step map which is not a problem as our system can easily be written in the same way. In fact the original 2-dimensional system came directly from second order one-dimensional system $\ddot{x} = ax^3 - bx$. Below we have (251) as a two step map (there is no need to look at the inverse as well):

$$\tilde{x} - 2x + \hat{x} = h^2(ax^3 - bx), \tag{253}$$

where $\hat{x} = x_{n-1}$.The classification of integrable difference equations includes a polynomial as the function on the right hand side like we have here, but it requires it to take the following form, where A, B, C, D, E are arbitrary constants:

$$\tilde{x} - 2x + \hat{x} = -h^2 \left(\frac{A + Bx + Cx^2 + Dx^3}{1 + h^2(E + \frac{Cx}{3} + \frac{Dx^2}{2})} \right). \tag{254}$$

Unfortunately our right hand side is lacking the denominator $1 - \frac{ah^2x^2}{2}$ to take the same form as (254), and therefore our discrete system is not integrable with a symmetric integral of the form:

$$J(x, y, h) = J_0(x, y) + h^2 J_1(x, y), \tag{255}$$

However this does not necessarily mean that our discretization is not at all integrable as it may well be but with a different non-symmetric integrator. We can quickly assess whether or not this is the case by performing the Diophantine test [19] which looks at the growth of the iterates.

6.6 Diophantine Test for Integrability

For this test we will be using the two-step version of the system, (253) and comparing it to a particular case of (254) which we already know is integrable. The particular case we will use here is the one which has the same numerator as (253):

$$\tilde{x} - 2x + \hat{x} = -h^2 \frac{ax^3 - bx}{1 + h^2 \frac{a}{2} x^2}. \tag{256}$$

We will be taking $a = \frac{1}{2}$ and $b = 1$. By using rational values for all inputs to these discrete systems we can measure the growth of the iterates numerically which will indicate whether the system is integrable or not. If we take each iterate $x_i = \frac{a_i}{b_i}$ to be a rational number then we can plot $\log(i)$ against $\log(\max\{a_i, b_i\})$ and then look to see whether the growth is exponential or similar to a polynomial, the latter of which being the indication of integrability.

First we will look at the system which we know to be integrable:

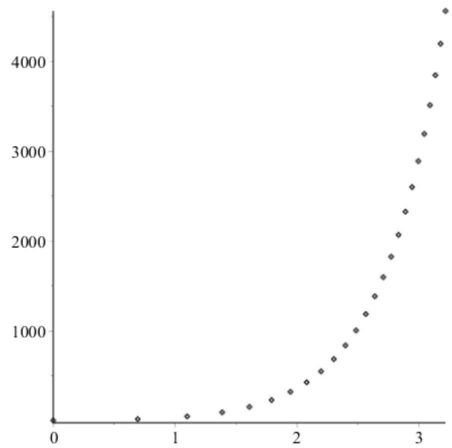

Figure 18: A plot of the growth of the heights of the iterates with $x_0 = \frac{1}{10}$, for the integrable system.

This plot shows the first 25 iterates of the system, and it can easily be seen that there is polynomial growth as we would expect. Now we can compare this to the plot for our system (253):

This time only 7 iterates have been plotted and already we can see the heights

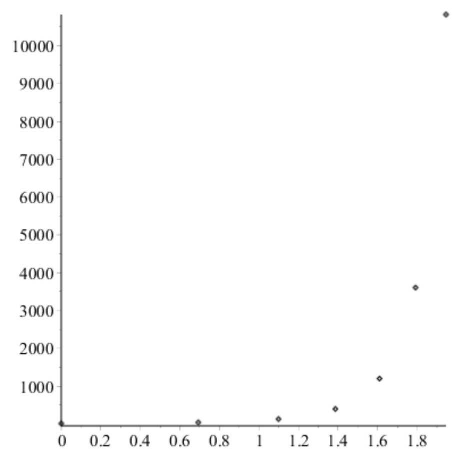

Figure 19: A plot of the growth of the heights of the iterates with $x_0 = \frac{1}{10}$, for the system (253).

of the iterates are growing exponentially which indicates that in fact this system is not integrable.

6.7 Conclusion

In the first part of this Chapter we use a similar method to that used in Chapter 3 to produce a generalisation of the Micken's type discretization scheme to discretize a cubic system that arises from a trimolecular system. Although this particular system had been discretized in the same way by Hone in [26], we took the generalisation further and included all possible parameters. Even with the inclusion of these extra parameters we did not find any new discrete maps for this system. We have begun to investigate the presence of a limit cycle in the discrete map (as is present the continous system) but further research into this and the exact bifurcation line for the discrete system is needed.

In the second part of the Chapter the same generalised discretization method is applied to a Hamiltonian system with a quartic potential, which was chosen due to the presence of elliptic orbits. This generalisation produces a single symplectic and birational map and its inverse, with only two of the five original parameters free to take any value. To investigate the integrability of this system we first compared it to a list of all integrable scalar difference equations that posseses a non-trivial symmetric integral [55] and we discovered that our system does not appear to be integrable, at least with the given integrator. We then used the Diophantine integrability test to investigate this further, and we found confirmation from this that the discrete map is indeed not integrable. This work could be extended by looking at other three-dimensional Hamiltonian system and looking for symplectic birational maps that are integrable, and to try to find out why exactly this method for producing discretizations does not always produce integrable maps.

Appendix A

Resultants

Resultants are used to determine whether two polynomials have a common root or not. For example, if we take two polynomials $P(x), Q(x)$ with degrees m and n respectively, and assume that they have a common root α. Let $P = \sum_{j=0}^{m} c_j x^j$ and $Q = \sum_{j=0}^{n} d_j x^j$ then we have the following matrix equation:

$$M \begin{pmatrix} \alpha^{m+n-1} & \alpha^{m+n} & . & . & . & \alpha & 1 \end{pmatrix}^T = \mathbf{0}, \tag{257}$$

with

$$M = \begin{pmatrix} c_m & c_{m-1} & c_{m-2} & ... & c_0 & 0 & ... & 0 \\ 0 & c_m & c_{m-1} & ... & c_1 & c_0 & ... & 0 \\ & & ... & . & . & . & . & . \\ 0 & 0 & . & . & . & . & . & c_0 \\ d_n & d_{n-1} & d_{n-2} & ... & d_0 & 0 & ... & 0 \\ 0 & d_n & d_{n-1} & ... & d_1 & d_0 & ... & 0 \\ & & ... & . & . & . & . & . \\ 0 & 0 & . & . & . & . & . & d_0 \end{pmatrix}. \tag{258}$$

Given that α is indeed a root of the two polynomial equations we then have $\mathbf{Det}(M) = 0$. This then becomes the condition to look for when working out if two polynomials have a common root. We will define the resultant as $R_{P,Q} = \mathbf{Det}(M)$.

Appendix B

Stability Analysis Example

In this example we will evaluate the stability of fixed points of a two-dimensional system and compare the classifications with the phase portrait to demonstrate the theory outlined previously.

Example 1. Given the following system of ODE's in the (x, y) plane

$$\dot{x} = xy + y, \qquad \dot{y} = x^2 - y^2 - 8x, \tag{259}$$

we can find the fixed points of the system by evaluating $\dot{x} = 0$ and $\dot{y} = 0$ simultaneously. The first equation gives the following two possibilities:

$$y(x+1) = 0, \implies y = 0 \quad \text{or} \quad x = -1. \tag{260}$$

Taking $y = 0$ from this and substituting into the second equation gives

$$x^2 - 8x = 0 \implies x = 0 \quad \text{or} \quad x = 8, \tag{261}$$

and therefore we have the first two fixed points, $(0,0)$ and $(8,0)$. Now taking $x=-1$ from the first equation we have

$$9-y^2=0 \implies y=3 \quad \text{or} \quad y=-3, \tag{262}$$

giving us the last two fixed points $(-1,3)$ and $(-1,-3)$. Now that we have established that this system has four fixed points, we can now perform stability analysis on them to find out how trajectories behave near each point. The Jacobian of the system needs to be calculated,

$$J=\begin{pmatrix} y & x+1 \\ 2x-8 & -2y \end{pmatrix}, \tag{263}$$

and then evaluated at each point to give the corresponding community matrix. We shall assign the fixed points as follows: $z_1^*=(0,0)$, $z_2^*=(8,0)$, $z_3^*=(-1,3)$ and $z_4^*=(-1,-3)$, and their corresponding community matrices as A_1, A_2, A_3, A_4.

$$A_1=\begin{pmatrix} 0 & 1 \\ -8 & 0 \end{pmatrix}, A_2=\begin{pmatrix} 0 & 9 \\ 8 & 0 \end{pmatrix}, A_3=\begin{pmatrix} 3 & 0 \\ -10 & -6 \end{pmatrix}, A_4=\begin{pmatrix} -3 & 0 \\ -10 & 6 \end{pmatrix}. \tag{264}$$

The eigenvalues for each matrix can now be calculated using (11) which gives the following characteristic equations:

$$\begin{aligned} z_1^* &: \lambda^2+8=0, & z_2^* &: \lambda^2-72=0, \\ z_3^* &: (3-\lambda)(-6-\lambda)=0, & z_4^* &: (-3-\lambda)(6-\lambda)=0. \end{aligned} \tag{265}$$

Finally these equations are solved to give two eigenvalues, and then Theorem 1.3 can be used to classify each fixed point.

$$\begin{aligned} z_1^* &: \lambda=\pm 2\sqrt{2}i: \text{ centre}, & z_2^* &: \lambda=\pm 6\sqrt{2}: \text{ saddle}, \\ z_3^* &: \lambda=3,-6: \text{saddle}, & z_4^* &: \lambda=-3,6: \text{saddle}. \end{aligned} \tag{266}$$

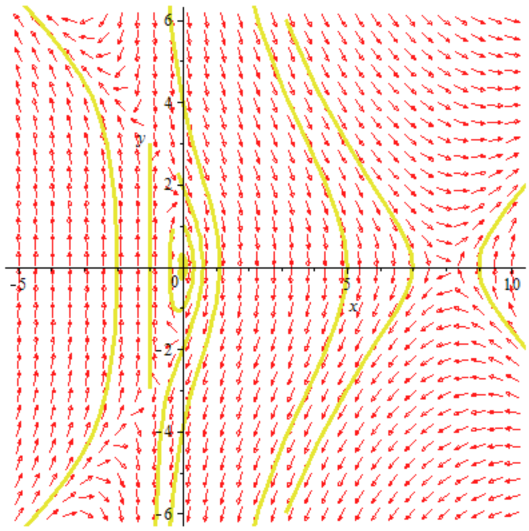

Figure 20: The phase space of the system (259).

These fixed points define the phase portrait which can be seen in figure 20 .

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