The Characteristics of Patterns in Simple Discrete Reaction-Diffusion Systems of Different Dimensionality and Number of Species

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Abstract

The formation of smooth quasi-periodic patterns in static discrete reaction-diffusion systems of various kinds is here studied from a mathematical point of view. The regularity of the patterns can be attributed to the integrability of the system, so that, when searching for such patterns in a system, it is important to investigate whether or not there exist any conserved quantities. The work presented herein is an attempt to generalize a known method, which finds a mathematical representation of the reaction mechanisms allowing for a conserved quantity in the one-dimensional one-species case. It is shown that although the method does not generalize to higher spatial dimensionality, it is possible to generalize to an arbitrary number of species in one dimension, where the reaction mechanism is a generalization of that found in the known method. A fixed-point relation for the system is found and analyzed for an arbitrary number of species, whereas the stabilities and other characteristics of the fixed-points are studied for the two-species case. Numerical simulations show that quasi-periodic patterns indeed can exist along the spatial dimension of the two-species system, and have characteristics that agree with the developed theory. The stabilities in time of these patterns are unclear, since a static case of the reaction-diffusion dynamics is studied. It should be noted that the static case investigated is not uniquely defined by reaction-diffusion dynamics, so that the patterns, if stable, might be found so under some dynamics other than reaction-diffusion.

Contents

1 Introduction

The structure of a pine cone and the stripes of a zebra are but two forms of what is commonly referred to as a pattern. The fact that patterns, to a high degree, are omnipresent in nature, has inspired many scientists to investigate the phenomenon of pattern generation. An example of such a scientist is Alan Turing with his work regarding pattern formation in so-called reaction-diffusion systems [4]. A reaction-diffusion system is a system where, e.g., chemical reactants are allowed to both diffuse and undergo chemical reactions with each other. The whole system can thus be described by a set of coupled reaction formulas, and Turing showed that the emergence of patterns depends on, among other things, the ratio between the substances' respective diffusion constants. Also, when the study of non-linear dynamics was further developed, it was possible to understand, for instance, the perplexing results of Belousov and Zhabotinsky, where in a chemical reaction, the BZ-reaction (named after its discoverers), oscillating patterns were observed to emerge.

Today, much research is done about plant phyllotaxis, i.e. the arrangements of plant organs, because the apparent patterns there are intriguing. An example of these intriguing patterns is that of the pine cone, where the Fibonacci series can be found when the spiral structure is investigated more closely. Due to the chemical nature of the growth process of a plant, reaction-diffusion systems are studied in particular. It is thought that the hormone auxin is one of the key components in such growth, so several models for the transport of this substance have been presented, see for example [2]. These biological scenarios are all ruled by the underlying mathematics, and the aim of this thesis is to investigate from a mathematical point of view the formation of patterns, and their characteristics, in discrete reaction-diffusion systems of different dimensionality and more general character.

1.1 A mathematical description

As the name suggests, a reaction-diffusion system should be possible to describe by a modified diffusion equation, where the modification incorporates the reaction mechanism. The diffusion equation for the variable[1] $u = u(\mathbf{x}, t)$, where $\mathbf{x} = (x_1, \ldots, x_n)$ is position in n-dimensional space and t is time, can in dimensionless variables be written

$$\frac{\partial u}{\partial t} = \nabla^2 u \tag{1}$$

where $\nabla^2 = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ is the Laplace operator. Now, adding the term $F(u)$, representing the sought reaction mechanism, yields the reaction-diffusion equation

$$\frac{\partial u}{\partial t} = \nabla^2 u + F(u) \tag{2}$$

For convenience, reaction-diffusion will in this report be abbreviated as RD.

[1] This variable might e.g. represent a concentration distribution.

If the function u is interpreted as that which can give rise to patterns in the system, e.g. as the concentration of auxin in a plant, the above equation can be further simplified. Patterns should be constant in time, so, if such are to form, then the partial time derivative of u in the RD-equation must vanish, thus giving the static RD-equation

$$0 = \nabla^2 u + F(u) \tag{3}$$

Discretizing space into an n-dimensional lattice, gives the discretized RD-equation

$$0 = \sum_{j \in \xi(i)} u_j - f\left(u_i\right) \tag{4}$$

where u_i is the variable at lattice point i, $\xi(i)$ is the set of all nearest neighbors of point i, and $f(u_i)$ is the discretized version of $F(u)$ together with the discretized parts of $\nabla^2 u$ not depending on nearest neighbors. (For a derivation of this equation, see app. A). As an example, for one dimension this equation becomes

$$0 = u_{i+1} + u_{i-1} - f\left(u_i\right) \equiv u_+ + u_- - f(u) \tag{5}$$

where a relative notation has been defined for convenience. $u_\pm$ are in this notation the nearest neighbors of $u \equiv u_i$, where $\pm$ indicates whether the neighboring point is in a positive or negative direction, i.e. $i \pm 1$.

In a conservative system, i.e. a system in which some quantity is conserved, patterns are particularly smooth and quasi-periodic, and thus different from patterns displaying e.g. chaotic behaviour [3]. The question is thus what $f(u)$ can look like for the system to obtain this property, and whether or not there are more than only one such conserved quantity. For the one-dimensional case, Söderberg [3] managed to find a family of functions f that allow for a conserved quantity. His method is reviewed in sec. 2, and forms the starting point of this project.

The goal is to see if it is possible to generalize the method to a higher number of independent variables (i.e., spatial dimensions) or a higher number of dependent variables (i.e. to make u a vector), and, if so, perform computer simulations to verify it. Increasing the number of dependent variables can be seen as looking at several chemical species reacting and diffusing in the system. One way to try to generalize the method for such many-species systems, would be to study whether or not conserved quantities can be found when $f(u)$ is some generalized vector field of the function found for the one-dimensional one-species case. The RD-equation for such a one-dimensional many-species system can be written, with a notation that is an obvious extension of that described earlier,

$$\mathbf{u}^+ + \mathbf{u}^- = \mathbf{f}(\mathbf{u}) \tag{6}$$

Throughout the report, the word *dimension* will refer to lattice dimension and the *number of components* and *species* will be used interchangeably for the number of components of the vector $\mathbf{u}$.

1.2 Structure

The report is divided into several sections, each of which may contain subsections. Because of the theoretical nature of the project, there are two theory sections: the first, called **The theoretical background** (sec. 2), presenting the general theory and Söderberg's method of solving the one-dimensional problem for one species, and the second, called **The theoretical analysis** (sec. 3), presenting the theoretical results obtained. After this, there is a section called **Results and discussion** (sec. 4), in which simulations are presented and analyzed. The last section, **Summary** (sec. 5), gives a brief summary of the work and speculations about what can be done in the future.

2 The theoretical background

This section is divided into two subsections. The first of these presents the general formulation of the problem for one species in a detailed manner, along with a few side-comments about that for an arbitrary number of species, whereas the second shows the known solution for the one-dimensional one-species case.

2.1 A general formulation of the problem

An RD-system for a single species at steady-state ($\partial_t u = 0$) can, as was shown in the introduction, be described by one of the equations

$$\begin{cases} 0 = \nabla^2 u + F(u) & (i) \\ 0 = \sum_{j\in\xi(i)} u_j - f(u_i) & (ii) \end{cases} \tag{7}$$

where (i) is for the continuous case and (ii) for the discrete case. These equations are throughout this section referred to as the *equations of motion* (EoM), even though the true equations of motion should be non-static, i.e. with $\partial_t u$ in the left-hand side.

A side-note is now in place: A Newtonian system with d degrees of freedom, i.e. a system on the form $\ddot{\mathbf{x}} = \mathbf{G}(\mathbf{x})$ (where $\mathbf{x}$ is a d-component position vector), can be rewritten as a Hamiltonian system of $2d$ variables (because a momentum vector $\mathbf{p} = m\dot{\mathbf{x}}$ has been defined). As should be noted, all of the d degrees of freedom depend on only one variable: time. The Newtonian mechanics hence define a flow in the $2d$-dimensional so called phase space spanned by the variables $\{x_i, p_i\}_{i\in\{1,2,\dots,d\}}$, see e.g. [1]. Now, there is an analogy between such systems and some of the RD-systems studied: the independent variables in the RD-system represent the dimensions of the lattice (analogous to time in the Newtonian system), whereas the dependent variables represent the different species (analogous to the position vector components in the Newtonian system), and if the RD-system studied is one-dimensional with N species, then the $2N$-dimensional phase space and the trajectories therein can be investigated[2].

[2]This is helpful since phase space contains much information, one example being the possibility to see whether or not conservation is possible from just the behaviours of trajectories. This will be discussed more thoroughly later in the report.

Now, the continuous system shows some interesting features which can be helpful when analyzing the discrete one. Therefore, the continuous case is reviewed first.

2.1.1 A continuous system

One way to obtain a smooth quasi-periodic pattern in a system[3], is to have some conserved quantity [3]. Conservation means that there must exist some non-trivial current $\mathbf{j}$ satisfying

$$0 = \nabla \cdot \mathbf{j} = \sum_{i=1}^{n} \partial_i j_i \tag{8}$$

where $\partial_i \equiv \frac{\partial}{\partial x_i}$ and $\mathbf{j} = (j_1, \ldots j_n)$. This can be seen as a Kirchhoff law, i.e., the sum of the flow in and out of each point must equal zero.

Now, if there exist several[4], $m \leq n$, say, conserved currents $\left\{\mathbf{j}^{(l)}\right\}_{l=1}^{m}$, there must be such a law for each l. For so-called *Noether-currents*, this conservation law can be shown to be,

$$\nabla \cdot \mathbf{j}^{(l)} = \partial_l u \cdot (\text{EoM}) \tag{9}$$

for dimensions $\{l\}$ [3]. Conserved Noether-currents can be found in systems with certain symmetries (as an example, a rotational symmetry corresponds to conservation of angular momentum and a translational symmetry to conservation of momentum). It is interesting to see whether or not such conservation laws are possible in an RD-system.

To investigate this, now assume that the function F from the EoM can be written as the derivative with respect to u of a potential $V(u)$ (with a minus sign), so that the EoM becomes

$$0 = \nabla^2 u - \frac{dV}{du} \tag{10}$$

Now consider translation symmetric and independent coordinate x_i. This leads to

$$0 = \partial_i u \cdot \left(\nabla^2 u - \frac{dV}{du}\right) = \partial_i u \cdot \left(\sum_{j=1}^{n} \frac{\partial^2 u}{\partial x_j^2} - \frac{dV}{du}\right) \tag{11}$$

However, this expression can be further simplified to

$$\begin{aligned} 0 &= \partial_i \left(\frac{1}{2}\left(\partial_i u\right)^2 - V(u) - \frac{1}{2}\sum_{j\neq i}\left(\partial_j u\right)^2\right) + \sum_{j\neq i}\partial_j\left(\partial_i u \cdot \partial_j u\right) = \\ &= \nabla \cdot \left(\partial_1 u \cdot \partial_i u\,, \ldots, \frac{1}{2}\left(\partial_i u\right)^2 - V(u) - \frac{1}{2}\sum_{j\neq i}\left(\partial_j u\right)^2, \ldots, \partial_n u \cdot \partial_i u\right) \equiv \\ &\equiv \nabla \cdot \mathbf{J}^{(i)} \end{aligned} \tag{12}$$

[3] The system is assumed, as before, to be n-dimensional, with spatial dimensions $\{x_i\}_{i\in\{1,\ldots,n\}}$

[4] Actually, it can be shown that, for a continuous system with a Lagrangian without explicit time-dependence, m must equal n. However, because of the analysis of the discrete system following shortly, let m still not necessarily equal n.

where in the last step the conserved Noether-current, $\mathbf{J}^{(i)}$, has been defined[5]. If the conserved quantity for one of the dimensions is defined as $\mathbf{J}^{(k)} = \left(j_1^{(k)}, \ldots, j_n^{(k)}\right)$, then the above conservation gives the requirement

$$0 = \nabla \cdot \mathbf{J}^{(k)} = \sum_{i=1}^{n} \partial_i j_i^{(k)} \tag{13}$$

which is the sought Kirchhoff law. Therefore, under some assumptions it is possible to find conserved quantities in continuous RD-systems.

2.1.2 A discrete system

Now that the continuous system has been analyzed, the discrete one is easily investigated. If there are to be m conserved quantities when the n-dimensional system is discretized, discretized versions of the Kirchhoff law above must be obeyed. Thus, in the same notation as above, with the derivatives ∂ changed to differences Δ, equations of the form

$$0 = \sum_{i=1}^{n} \Delta_i \, j_i^{(l)}(\mathbf{k}) \tag{14}$$

must be satisfied at each lattice point $\mathbf{k} = (k_1, k_2, \ldots, k_n)$ for all m dimensions $\{l\}$. Here, $\Delta_i \, j_i^{(l)}(\mathbf{k}) \equiv j_i^{(l)}(\mathbf{k} + \mathbf{e}_i) - j_i^{(l)}(\mathbf{k}) \equiv j_i^{(l)}(k_1, \ldots, k_i + 1, \ldots, k_n) - j_i^{(l)}(k_1, k_2, \ldots, k_n)$, or, in other words, it subtracts the value of $j_i^{(l)}$ at point $\mathbf{k}$ from its value at point $\mathbf{k} + \mathbf{e}_i$, i.e. the same point one step ahead in direction i.

As an example, consider a one-dimensional system. Discretize space into a line where the position on the line is denoted by k. Defining $j_1^{(l)}(k) \equiv j(k)$ as a flux between points $k-1$ and k, and $\Delta_1 \, j(k) \equiv j(k+1) - j(k)$ gives the requirement

$$0 = j(k+1) - j(k) \tag{15}$$

This really is a Kirchhoff law, since the flux between points $k+1$ and k must equal that between k and $k-1$ (the negative sign comes from the direction of the flux) so that no net "charge" piles up at point k.

For the RD-system, look at the quantity u defined earlier. The EoM for the discrete system of n dimensions is

$$0 = \sum_{j \in \xi(i)} u_j - f\left(u_i\right) \tag{16}$$

Now, in analogy with the continuous case, conserved quantities $\left\{\mathbf{J}^{(l)}\right\}$ are sought. The maximum number[6] of independent conserved quantities in a system is equal to the number of degrees of freedom [3], and if all of them exist, the system is said to be *integrable* [1].

[5] In a more compact notation the Noether-current can be written as $J_k^{(i)} = \partial_i u \, \partial_j u - \delta_{ik} \left(\frac{1}{2} \sum_l (\partial_l u)^2 + V(u) \right)$, where δ_{ik} is the Kronecker delta.

[6] Ignoring the trivial cases, that is.

Conservation for the one-dimensional system of one species

Also for a discrete system, a phase space can be defined. As an example, the EoM for a one-dimensional system of one species can be written, in a relative notation,

$$0 = u_+ + u_- - f(u) \tag{17}$$

which is a discrete Newtonian system. Defining $u_- \equiv t$ gives a mapping $T_2 : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$, i.e. $(u, t) \mapsto (u_+, t_+)$, explicitly written as

$$T_2 : \begin{cases} u_+ = & f(u) - t \\ t_+ = & u \end{cases} \tag{18}$$

and as can be seen, this is a discrete Hamiltonian system of two variables. Therefore, phase space is two-dimensional and spanned by $(u, t) = (u, u_-)$, and if there exists a conserved quantity, $H(u, t)$, say, it must be conserved along a trajectory in this space. That the quantity is conserved along a trajectory requires that

$$H(u_+, u) = H(u, u_-) \tag{19}$$

for all lattice points. The conserved quantity can be either symmetric or anti-symmetric, but if only symmetric quantities are sought, $H(u_+, u) = H(u, u_+)$ must be satisfied for all lattice points.

A summary of the requirements on the sought conserved quantity in the one-dimensional system therefore is:

1. Conservation means that an equation of the form $0 = \Delta_1 j_1(\mathbf{k})$, i.e. a generalized discrete continuity equation, is fulfilled. This means that a conserved quantity H satisfies $0 = \Delta H \equiv H_+ - H$, where the subscript $+$ is used in the same way as before.
2. The conserved quantities must be conserved along trajectories in the phase space spanned by $(u, u_-) = (u, t)$.
3. The conserved quantities must be symmetric functions of their respective arguments.

A side note on the higher-dimensional system of one species

In higher-dimensional systems the solutions are no longer one-dimensional trajectories in phase space, since there is more than one independent variable.

Phase space characteristics for conservative systems of one dimension and an arbitrary number of species

The phase space characteristics for discrete conservative systems is quite different from that of discrete dissipative systems, so a brief description of the behavior that can be expected in the conservative case is in place. The reason for this importance is, that in order to say whether or not there are conserved quantities in the investigated RD-systems, the numerically created trajectories must display certain characteristics[7].

[7]The exact characteristics vary with phase space dimensionality, but these characteristics are essential for all conservative systems.

1. *Types of fixed points under the mapping*[8]*:* Phase space volume is constant, i.e. there can be no pure attractors or repellers. Therefore, saddle-points (often called *hyperbolic* fixed points) and centers (often called *elliptic* fixed points) are the only options. That phase space volume is constant is equivalent to the mapping's Jacobian, $\mathbf{J}$, satisfying[9] $\det \mathbf{J} = 1$, which in turn means that its eigenvalues, $\{\lambda_j\}$, satisfy $\prod_j \lambda_j = 1$ (see e.g. [1]).
2. *Trajectories:* The trajectories can be either periodic, quasi-periodic or chaotic (see e.g. [1]).
3. *Chaos:* If there is chaotic behaviour in the system, the system is not integrable (see e.g. [1]).

2.2 The known method for the one-dimensional system of one species

Here, a brief overview of the existing method (see [3]) to find $f(u)$ allowing for a conserved quantity $H(u, u_-)$ is presented for the one-dimensional static discrete RD-system of one species. Such a system is described by the EoM

$$u_+ + u_- = f(u) \tag{20}$$

The conserved quantity $H(u, u_-)$ has to satisfy $H(u_+, u) = H(u, u_-) = H(u_-, u)$, i.e., it has to be conserved and symmetric. Multiplying the EoM with the discretized derivative $\Delta u = (u_+ - u_-)$, in analogy with equation 9, gives

$$(u_+ - u_-)(u_+ + u_- - f(u)) = 0 \tag{21}$$

Simplifying this expression and collecting terms of similar subscript on the same side of the equality yields

$$u_+^2 - u_+ f(u) = u_-^2 - u_- f(u) \tag{22}$$

It is possible to add an arbitrary function $g(u)$ on both sides and multiply by an arbitrary function $h(u)$. Doing this gives

$$h(u)\left(u_+^2 - u_+ f(u) + g(u)\right) = h(u)\left(u_-^2 - u_- f(u) + g(u)\right) \tag{23}$$

Now, assume that the arbitrary functions are such that the resultant expression, because of the sought properties of H, becomes

$$\begin{aligned} H(u_+, u) &\equiv A u_+^2 u^2 - B\left(u_+^2 u + u_+ u^2\right) + C\left(u_+^2 + u^2\right) + D u_+ u - E(u_+ + u) = \\ &= A u_-^2 u^2 - B\left(u_-^2 u + u_- u^2\right) + C\left(u_-^2 + u^2\right) + D u_- u - E(u_- + u) \equiv \\ &\equiv H(u, u_-) \end{aligned} \tag{24}$$

where A, B, C, D and E are constants. Note that this equality is a conservation law, symmetric in its arguments on the respective sides of the equality, hence the definitions of $H(u_+, u)$ and $H(u, u_-)$. Redefining these as $H_+ \equiv H(u_+, u)$

[8] See eq. (44).

[9] This is easily checked for the mapping in eq. (18). Since phase space is two-dimensional, the mapping is called *area-preserving*.

and $H \equiv H(u, u_-)$, and then subtracting the right hand side from the left hand side, gives a discretized derivative $\Delta H \equiv H_+ - H = 0$ as was sought. It thus has been shown that it in one dimension is possible to obtain a conserved quantity along all trajectories in phase space. However, $f(u)$ still remains to be found, something which is easily done by rewriting the conservation law above. Putting all terms of degree two in $u_\pm$ on the left hand side, and those of degree one on the right hand side, gives

$$\left(u_+^2 - u_-^2\right)\left(Au^2 - Bu + C\right) = \left(u_+ - u_-\right)(Bu^2 - Du + E\right) \tag{25}$$

Factorizing the difference of squares on the left, canceling mutual factors and dividing by the second degree polynomial of the left hand side[10] yields

$$u_+ + u_- = \frac{Bu^2 - Du + E}{Au^2 - Bu + C} \equiv f(u) \tag{26}$$

where the function $f(u)$ has been defined in the last step. Note that one of the constants, B, is present in both numerator and denominator. To conclude, a conserved symmetric quantity was found for a family of functions $\{f\}$.

3 The theoretical analysis

In this section the novel theoretical work is presented. It is divided into two parts, the first where the variable u is considered a scalar, and the second where it is instead considered a vector.

3.1 The scalar field

Here, the variable u is assumed to be a scalar, i.e. the number of species is equal to one. The section is divided into parts according to the different dimensionalities of the systems analyzed.

3.1.1 Perturbing the one-dimensional system

As was shown earlier, a family of functions $f(u)$ could be found along with corresponding conserved quantities for the one-dimensional system. Before going on to higher dimensions it can be interesting to see what trajectories in phase space look like for the one-dimensional case. Also, because of the relation between coefficients in the rational polynomial f, it is of particular interest to see what happens to the dynamics if the relation is changed by some perturbation. This can be done by letting a computer perform the iterated mapping

$$T_2 : \begin{cases} u_+ = & f(u) - t \\ t_+ = & u \end{cases} \tag{27}$$

for both the unperturbed system and for the perturbed, and then plot the respective sets of trajectories in (u_+, u), where in the mapping $u_- \equiv t$. The perturbed

[10] This imposes the restriction that the constants A, B and C be chosen such that not all three are zero at the same time.

system then should show non-conservative behaviour, by e.g. displaying chaos. The results of this are shown in app. C.

3.1.2 Two dimensions and higher

Now, consider the two-dimensional case. The EoM are thus, for the set of nearest neighbours $\xi(i)$,

$$0 = \sum_{j \in \xi(i)} u_j - f(u_i) \tag{28}$$

If the system is defined on a square lattice, i.e. each point has four nearest neighbours, the sum consists of four terms for each point on the lattice. In analogy with the x- and y-axes in the Cartesian plane, let the system be defined in terms of two orthogonal coordinate axes, x_1 analogous to x and x_2 analogous to y, so that u needs two labels to be defined. Let $u \longrightarrow u_{ij}$ where i corresponds to x_1 and j to x_2. The indices $i, j \in \mathbb{Z}$, but for notational convenience, let i and j be expressed in a relative notation by belonging to the set $\{-, 0, +\}$, i.e. for each point the associated nearest neighbors are referred to in terms of positions relative to the point itself (just like the index for the one-dimensional discrete system). As a special case, let $u_{00} \equiv u$. This gives the EoM

$$0 = u_{+0} + u_{-0} + u_{0+} + u_{0-} - f(u) \tag{29}$$

Now, if the system is integrable there have to be two non-trivial constants of the motion. These should be possible to derive from the Noether conservation identities

$$\begin{cases} 0 = \nabla \cdot \mathbf{J}^{(1)} \equiv \Delta_1 j_1^{(1)} + \Delta_2 j_2^{(1)} \stackrel{?}{=} (u_{+0} - u_{-0}) \cdot (\text{EoM}) \\ 0 = \nabla \cdot \mathbf{J}^{(2)} \equiv \Delta_1 j_1^{(2)} + \Delta_2 j_2^{(2)} \stackrel{?}{=} (u_{0+} - u_{0-}) \cdot (\text{EoM}) \end{cases} \tag{30}$$

where the superscript $m \in \{1, 2\}$ denotes which of the conserved quantities is investigated, and $\mathbf{J}^{(m)} = (j_1^{(m)}, j_2^{(m)})$. The question marks show that it is not certain whether or not the equalities actually hold, rather that it is a guess analogous to the continuous case (cf. equation 9). Because of the symmetry of axis choice, it suffices to investigate one of the conserved quantities. For conserved quantity *2* this becomes

$$\begin{aligned} 0 &= (u_{0+} - u_{0-}) \cdot (u_{+0} + u_{-0} + u_{0+} + u_{0-} - f(u)) = \\ &= u_{0+}^2 - u_{0-}^2 + u_{0+}u_{+0} + u_{0+}u_{-0} - u_{0-}u_{-0} - u_{0-}u_{-0} + \\ &\quad -u_{0+}f(u) + u_{0-}f(u) \end{aligned} \tag{31}$$

Now assume that $f(u)$ can be written as $P(u)/Q(u)$, where P and Q are so far arbitrary functions. The equation can now be multiplied by $Q(u)$, yielding

$$\begin{aligned} 0 &= u_{0+}^2 Q(u) - u_{0-}^2 Q(u) + u_{0+}u_{+0}Q(u) + u_{0+}u_{-0}Q(u) + \\ &\quad -u_{0-}u_{+0}Q(u) - u_{0-}u_{-0}Q(u) - u_{0+}P(u) + u_{0-}P(u) \end{aligned} \tag{32}$$

This expression has to be possible to write as a sum of differences. Rearranging the expression in terms of $u_{0\pm}$ gives

$$\begin{aligned} 0 &= \left[u_{0+}^2 Q(u) + u_{0+}u_{+0}Q(u) + u_{0+}u_{-0}Q(u) - u_{0+}P(u)\right] + \\ &\quad + \left[-u_{0-}^2 Q(u) - u_{0-}u_{+0}Q(u) - u_{0-}u_{-0}Q(u) + u_{0-}P(u)\right] \end{aligned} \tag{33}$$

What can now be noted is that if $f(u)$ is linear[11] in u, i.e. $Q(u)$ can be chosen as constant and $P(u) \sim u$, then the expression can be written as a sum of differences, by adding and subtracting convenient terms, i.e. a symmetric conservation law exists, as sought. However, if $f(u)$ is assumed to be written as a polynomial fraction this is impossible. The problem arises with the terms $u_{0\pm}u_{\pm 0}Q(u)$ (over all combinations of $\pm$), to which no terms can be added and subtracted to give the sought property of the equation. For a cubic lattice in three dimensions the result must be the same.

This means that it is *impossible* to generalize the one-dimensional method for non-linear f to higher spatial dimensionality.

3.2 The vector field

Because of the impossibility of generalizing the one-dimensional method for one species to higher dimensions, now consider the case $u \longrightarrow \mathbf{u}$, i.e. let u instead be an N-component vector $\mathbf{u}$, still, however, on a one-dimensional lattice. A possible physical interpretation of the change from scalar to vector is to, instead of just looking at one chemical substance diffusing and reacting in a system, consider a system of N different chemical substances (the so-called species) which can diffuse and react with each other. Of course, not all substances need react with every other substance, but there must exist at least one such reaction for each substance (otherwise it would just be the same situation as before: an RD-system of several species independent of each other). The EoM can be written in vector form as

$$\mathbf{u}^+ + \mathbf{u}^- = \mathbf{f}(\mathbf{u}) \tag{34}$$

and in component form, for $i, j \in \{1, 2, \ldots, N\}$,

$$u_i^+ + u_i^- = f_i\left(\{u_j\}\right) \tag{35}$$

The question is now if it is, in the spirit of the one-dimensional scalar case, possible to find a conserved quantity if $\mathbf{f}$ is chosen as some vector field, that is a generalized version of the family of functions f found in the known method, for a scalar variable, presented earlier. In component form this vector field can be written as

$$f_i(\mathbf{u}) = \frac{\tilde{B}_{i,kl}u_k u_l - D_{i,k}u_k + e_i}{A_{kl}u_k u_l - B_k u_k + C} \tag{36}$$

where the convention of summation over repeated indices is used. As the notation implies, a variable with no index is a scalar, with one index a vector, with two unseparated indices a matrix and otherwise some tensor of another rank. Note that the exact relation between $\tilde{B}_{i,kl}$ and B_k is not yet determined (cf. the one-dimensional case, eq. (26), where the B's were equal).

In analogy with the one-dimensional scalar case, a conserved quantity H that satisfies

$$\begin{cases} 0 \equiv \Delta H \equiv H\left(\mathbf{u}^+, \mathbf{u}\right) - H\left(\mathbf{u}, \mathbf{u}^-\right) \equiv \left(\mathbf{u}^+ - \mathbf{u}^-\right) \cdot (\text{EoM}) \\ H\left(\mathbf{u}^+, \mathbf{u}\right) = H\left(\mathbf{u}, \mathbf{u}^+\right) \end{cases} \tag{37}$$

[11] A trivial case, since this would represent pure diffusion.

is now sought, where "$\cdot$" is now a generalized scalar product defined, for vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^N$ and a positive-definite symmetric matrix $\mathbf{G} \in \mathbb{R}^{N\times N}$ (the "metric tensor"), as $\mathbf{a}\cdot\mathbf{b} \equiv a_i G_{ij} b_j$. Performing the operation gives, in component form,

$$0 = \left(u_j^+ - u_j^-\right) G_{ij} \left(u_i^+ + u_i^- - f_i(\mathbf{u})\right) \tag{38}$$

Using the expression for f_i and collecting terms of similar superscript ($\pm$) on either side of the equality then yields

$$\begin{aligned} &G_{ij}A_{kl}u_j^+u_i^+u_ku_l - G_{ij}B_ku_i^+u_j^+u_k + CG_{ij}u_j^+u_i^+ + \\ &-G_{ij}\tilde{B}_{i,kl}u_ku_lu_j^+ + G_{ij}D_{i,k}u_j^+u_k - e_iG_{ij}u_j^+ = (+ \longrightarrow -) \end{aligned} \tag{39}$$

Note that this resembles a conservation law, the difference being that it in its current form is not symmetric. For both the left-hand side and the right-hand side to be symmetric in their respective arguments, the following conditions must be satisfied:

1. $G_{ij}A_{kl} = G_{kl}A_{ij}$
2. $G_{ij}D_{i,k} = G_{ik}D_{i,j} = G_{ki}D_{i,j}$ (The last equality follows from the restriction that G be symmetric)
3. $B_k = G_{kl}b_l$ and $\tilde{B}_{l,ij} = b_lG_{ij}$
4. An appropriate function of $\mathbf{u}$ is added on both sides.

The implications of these conditions are:

Condition 1 For a fixed pair ij, $G_{kl} = A_{kl}\frac{G_{ij}}{A_{ij}} \propto A_{kl}$, $\forall k, l$. Therefore, let $\mathbf{A} = a\mathbf{G}$ where a is some constant.

Condition 2 This is just symmetric matrix multiplication, i.e. $\mathbf{GD}$ is a symmetric matrix. Denoting this product as $\mathbf{S}$ gives $\mathbf{GD} = \mathbf{S}$. Assuming that $\mathbf{G}$ is non-degenerate[12], $\mathbf{D}$ can be written as $\mathbf{D} = \mathbf{G}^{-1}\mathbf{S}$. If $\mathbf{S}$ is now written as the symmetric combination $\mathbf{S} = \mathbf{GS'G}$, where $\mathbf{S'}$ is some other symmetric matrix, $\mathbf{D}$ becomes $\mathbf{D} = \mathbf{S'G}$. Since both $\mathbf{S}$ and $\mathbf{S'}$ are arbitrary names, $\mathbf{S'}$ can be redefined to give $\mathbf{D} = \mathbf{SG}$. In component form, $D_{i,k} = S_{il}G_{kl}$.

Condition 3 This condition, along with the preceding two, gives $f_i(\mathbf{u})$ as

$$f_i(\mathbf{u}) = \frac{b_iG_{kl}u_ku_l - S_{il}G_{kl}u_k + e_i}{aG_{kl}u_ku_l - b_lG_{kl}u_k + C} \tag{40}$$

As can be seen when compared to the original structure in eq. (36), the relation between $\tilde{B}_{i,kl}$ and B_k is very similar to that in the scalar case (see eq. (26)).

Condition 4 The terms that need to be added for the expression to be completely symmetric are $CG_{ij}u_ju_i - G_{ij}e_iu_j$.

Using the above conditions, the conservation law becomes

$$\begin{aligned} &aG_{ij}G_{kl}u_j^+u_i^+u_ku_l - G_{ij}G_{kl}b_lu_i^+u_j^+u_k + CG_{ij}\left(u_j^+u_i^+ + u_ju_i\right) + \\ &- G_{ij}G_{kl}b_iu_ku_lu_j^+ + G_{ij}S_{il}G_{kl}u_j^+u_k - e_iG_{ij}\left(u_j^+ + u_j\right) = \\ &= (+ \longrightarrow -) \end{aligned} \tag{41}$$

[12]That a matrix is non-degenerate is equivalent to the existence of its inverse, which in turn is equivalent to the matrix having full rank, which in turn is equivalent to having determinant not equal to zero. In mathematics, for $N\times N$-matrix $\mathbf{G}$ and $N\times N$-unit matrix $\mathbf{1}$; $\mathbf{G}$ non-deg. $\Leftrightarrow$ $\exists\mathbf{G}^{-1}$: $\mathbf{G}^{-1}\mathbf{G} = \mathbf{G}\mathbf{G}^{-1} = \mathbf{1}$ $\Leftrightarrow$ $\mathrm{Rnk}(\mathbf{G}) = N$ $\Leftrightarrow$ $\det\mathbf{G} \neq 0$

Note that this expression now is symmetric under $\mathbf{u}^{\pm} \to \mathbf{u}$. Therefore, define the quantity on the left hand side as $H(\mathbf{u}^+, \mathbf{u})$ and that on the right as $H(\mathbf{u}, \mathbf{u}^-)$, so that $H(\mathbf{u}^+, \mathbf{u}) = H(\mathbf{u}, \mathbf{u}^-) = H(\mathbf{u}^-, \mathbf{u})$, as was sought. For arbitrary vectors $\mathbf{u}, \mathbf{t} \in \mathbb{R}^N$, the conserved quantity $H(\mathbf{u}, \mathbf{t})$ can be written

$$\begin{aligned} H(\mathbf{u}, \mathbf{t}) &= a\,\mathbf{u}^\top \mathbf{G}\mathbf{u}\,\mathbf{t}^\top \mathbf{G}\mathbf{t} - \mathbf{u}^\top \mathbf{G}\mathbf{u}\,\mathbf{b}^\top \mathbf{G}\mathbf{t} - \mathbf{t}^\top \mathbf{G}\mathbf{t}\,\mathbf{b}^\top \mathbf{G}\mathbf{u} + \\ &\quad + C\left(\mathbf{u}^\top \mathbf{G}\mathbf{u} + \mathbf{t}^\top \mathbf{G}\mathbf{t}\right) + \mathbf{u}^\top \mathbf{G}\mathbf{S}\mathbf{G}\mathbf{t} - \mathbf{e}^\top \mathbf{G}\left(\mathbf{u} + \mathbf{t}\right) \end{aligned} \tag{42}$$

It has thus been shown that there exists, in the investigated kind of system, at least one conserved quantity for each $\mathbf{f}(\mathbf{u})$ on the form of eq. (40). The EoM for the system can in vector form be written as

$$\mathbf{u}^+ + \mathbf{u}^- = \mathbf{f}(\mathbf{u}) \equiv \frac{\mathbf{b}\,\mathbf{u}^\top \mathbf{G}\mathbf{u} - \mathbf{S}\mathbf{G}\mathbf{u} + \mathbf{e}}{a\,\mathbf{u}^\top \mathbf{G}\mathbf{u} - \mathbf{b}^\top \mathbf{G}\mathbf{u} + C} \tag{43}$$

where the connection between choices of vector names and the expression for $f_i(\mathbf{u})$ in eq. (40) should be obvious.

The EoM can be rewritten as the $2N$-dimensional mapping $T : \mathbb{R}^{2N} \longrightarrow \mathbb{R}^{2N}$, or $(\mathbf{u}, \mathbf{t}) \mapsto (\mathbf{u}^+, \mathbf{t}^+)$,

$$T : \begin{cases} \mathbf{u}^+ = \mathbf{f}(\mathbf{u}) - \mathbf{t} \\ \mathbf{t}^+ = \mathbf{u} \end{cases} \tag{44}$$

where $\mathbf{t} \equiv \mathbf{u}^-$. Phase space is spanned by the variables $\{\mathbf{u}, \mathbf{t}\}$. Since one conserved quantity has been found, all trajectories must lie on the $(N-1)$-dimensional hypersurface in phase space defined by the value of the conserved quantity found[13]. The dynamics of this system are now to be investigated, as well as the possibility of patterns and their connection to phase space characteristics (e.g. fixed points and corresponding stabilities). This will be done by looking at the N-dimensional case for a while longer, after which, for simplicity, the $(N = 2)$-case is investigated more in-depth.

3.2.1 Diagonalization, rotation and translation

The very general structure of the vector field $\mathbf{f}(\mathbf{u})$ defined in eq. (43) can be further simplified. The following operations can be done to simplify $\mathbf{f}(\mathbf{u})$:

1. Diagonalize $\mathbf{G}$, by choosing a new basis in $\mathbf{u}$-space, and rescale $\{u_i\}$ relative to one another so that $\mathbf{G} \to \mathbf{1}$, where $\mathbf{1}$ is the unit matrix of size $N \times N$.
2. Rotate the new basis so that $\mathbf{S}$ becomes a diagonal matrix.
3. If $a \neq 0$, redefine variables so that a disappears from the expression. This is equivalent to putting $a = 1$ in the already existing expression.
4. Translate $\mathbf{u}$-space such that $\mathbf{u} \to \mathbf{u} + \frac{1}{2}\mathbf{b}$. This gives the new EoM as $\mathbf{u}^+ + \mathbf{u}^- + \mathbf{b} - \mathbf{f}\left(\mathbf{u} + \frac{1}{2}\mathbf{b}\right) = 0$. Simplifying this expression and redefining the variables yet again gives back the original EoM except for no $\mathbf{b}$'s in $\mathbf{f}(\mathbf{u})$, i.e. the linear term, in $\mathbf{u}$, in the denominator and the quadratic term, in $\mathbf{u}$, in the numerator have vanished.

[13] This is just like planetary orbits, confined to a plane, that move along curves of constant energy (given that the motions of planets are not chaotic).

Doing all of the above results in the much simpler expression

$$\mathbf{f}(\mathbf{u}) = \frac{-\mathbf{S}\mathbf{u} + \mathbf{e}}{\mathbf{u}^\top \mathbf{u} + C} \tag{45}$$

where $\mathbf{S}$ is diagonal, and hence the EoM

$$\mathbf{u}^+ + \mathbf{u}^- = \frac{-\mathbf{S}\mathbf{u} + \mathbf{e}}{\mathbf{u}^\top \mathbf{u} + C} \tag{46}$$

The conserved quantity then becomes

$$H(\mathbf{u}, \mathbf{v}) = \mathbf{u}^\top \mathbf{u}\, \mathbf{v}^\top \mathbf{v} + C\left(\mathbf{u}^\top \mathbf{u} + \mathbf{v}^\top \mathbf{v}\right) + \mathbf{u}^\top \mathbf{S}\mathbf{v} - \mathbf{e}^\top (\mathbf{u} + \mathbf{v}) \tag{47}$$

3.2.2 Fixed points of the mapping

As was stated earlier, a good starting point to understand the perhaps possible patterns is to study the fixed points of the mapping and their respective stabilities (under the mapping). The reason for this is that at a fixed point, there can be no pattern: A fixed point of the system, $(\mathbf{u}^*, \mathbf{t}^*)$, is such that T maps the point to itself, i.e. $T : (\mathbf{u}^*, \mathbf{t}^*) \mapsto (\mathbf{u}^*, \mathbf{t}^*)$ (or, in other words, the value is constant under the mapping). However, at small distances from elliptic fixed points, (quasi)-periodic patterns should occur [3]. At the fixed point the mapping requirement is thus, from eq. (44),

$$T : \begin{cases} \mathbf{u}^* = \mathbf{f}(\mathbf{u}^*) - \mathbf{t}^* \\ \mathbf{t}^* = \mathbf{u}^* \end{cases} \tag{48}$$

As can be seen, this condition can be rewritten as

$$2\mathbf{u}^* = \mathbf{f}(\mathbf{u}^*) = \frac{-\mathbf{S}\mathbf{u}^* + \mathbf{e}}{\mathbf{u}^{*\top}\, \mathbf{u}^* + C} \tag{49}$$

For notational convenience, let $\mathbf{u}^* \equiv \mathbf{u}$ and $\mathbf{u}^\top \mathbf{u} \equiv R$. This gives, in component form, upon rearrangement of the fixed point condition

$$(2R + S_{ii} + 2C)\, u_i = e_i \tag{50}$$

since $\mathbf{S} = \mathrm{diag}(S_{11}, \ldots, S_{NN})$. Now, there are two important cases[14] (i) $e_i \neq 0$ $\forall i$, and (ii) $e_i = 0$ $\forall i$.

Case (i)

Rearranging eq. (50) and using the definition of R yields

$$\begin{cases} u_i = \frac{e_i}{2(R+C)+S_{ii}} \equiv \frac{e_i}{2R-Q_i}\,, & \forall i \in \{1, 2, \ldots, N\} \\ R = \sum_{i=1}^N \frac{e_i^2}{(2(R+C)+S_{ii})^2} \equiv \sum_{i=1}^N \frac{e_i^2}{(2R-Q_i)^2} \end{cases} \tag{51}$$

where $Q_i \equiv -S_{ii} - 2C$. Note that the equation for R is actually of degree $2N + 1$, so that there can exist at most $2N + 1$ fixed points (which may be

[14] There is also the case where some components satisfy case (i) and the other case (ii). However, these are neglected here.

degenerate) for the system. Once $\{R^\alpha\}_{\alpha\in\{1,2,\dots,2N+1\}}$ and $\{e_i, Q_i\}_{i\in\{1,2,\dots,N\}}$ are known, the corresponding fixed points with components $\{u_i^\alpha\}$ are easily found. There are $2N^2+N$ such components. Finding $\{R^\alpha\}$ is equivalent to finding the intersections between the functions $y=R$ and $y=\sum_{i=1}^{N}\frac{e_i^2}{(2R-Q_i)^2}\equiv h(R)$ in the (y,R)-plane, see fig. 1.

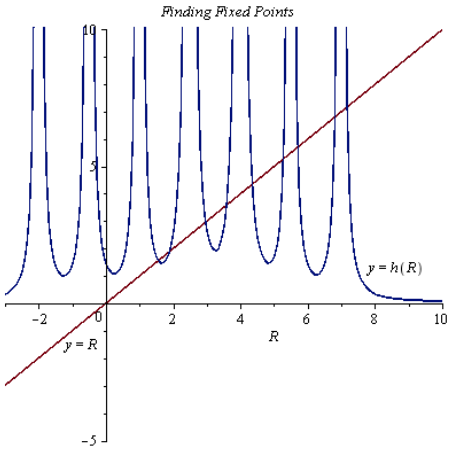

Figure 1: Intersections between $y=R$ and $y=h(R)$ (defined in the text) in the (y,R)-plane for a system with $N=7$. It should be noted that with $N=7$, the maximum number of fixed points should be 15, which may be degenerate (degeneracy for fixed points graphically means that the line $y=R$ is tangent to $y=h(R)$ at a point), and as the plot clearly shows, there are 9 distinct values of R for each of which there exists at least one fixed point. Here, the values of $\{e_i, Q_i\}$ have been chosen to best show the general behaviour.

Case (ii)

Case (ii) instead gives the condition

$$(2R+\mathbf{S}+2C)\,\mathbf{u}=\mathbf{0} \tag{52}$$

or, in component form,

$$(2R+S_{ii}+2C)\,u_i=0 \quad \forall i \tag{53}$$

From this condition the following can be said:

1. $u_i=0\ \forall i\in\{1,2,\dots,N\}\equiv\mathbb{A}$ always satisfies the relation, i.e. the origin is always a fixed point. For this there need not be any relations between S_{ii}, C and R.
2. If there exist fixed points for which some of the $j\in\mathbb{A}:\ u_j\neq 0$, then S_{jj} must satisfy $S_{jj}=-2C-2R$, or, equivalently, $S_{jj}=S_{kk}\ \forall j,k:\ u_j,u_k\neq 0$. This means that hyper-spheres of radii $R=-C-\frac{1}{2}S_{jj}$ with fixed points exist. Note, however, that if only one $j:\ u_j\neq 0$ exists (and all of the S_{ii} are different), then $u_j=\pm\sqrt{R}=\pm\sqrt{-C-\frac{1}{2}S_{jj}}$, which means

that there are two fixed points on each axis of the coordinate system and one in the origin, i.e. in total $2N+1$ fixed points[15].

Throughout the rest of this section, the special case where $N = 2$, i.e. the two-species case, is studied. In particular it is studied how to find the fixed points for cases (i) and (ii), as well as the general characteristics of the sought patterns. Also, the conserved quantity is investigated more in-depth.

3.2.3 A system of two-component vectors: Case (i)

Now, since $N = 2$ there must be five values of R, i.e. $\alpha \in \{1, 2, 3, 4, 5\}$, and ten components in total of the five two-component fixed points. There are several ways to find the fixed points. First of all, note that there are five free parameters so far: e_1, e_2, S_{11}, S_{22} and C. The fixed points obviously depend on the parameters chosen, and one way to find them is to choose $\{R^\alpha\}$ and calculate the rest that is needed with the fixed point relations presented in the previous section. The method adapted here is yet another, where two of the fixed points are *chosen*. Why only two are chosen and not for instance three, is because there only are five free parameters (unlike the six components of three fixed points). Before these are chosen numerically, $\{e_i, Q_i\}_{i\in\{1,2\}}$ are to be calculated. Let the chosen fixed points be $\left(u_1^1, u_2^1\right)$ and $\left(u_1^2, u_2^2\right)$, where the superscripts are equivalent to the index α.

Using the fixed point relation gives the set of equations, for $\alpha = 1, 2$,

$$\begin{cases} u_1^1 = \frac{e_1}{2R^1 - Q_1} \\ u_2^1 = \frac{e_2}{2R^1 - Q_2} \\ u_1^2 = \frac{e_1}{2R^2 - Q_1} \\ u_2^2 = \frac{e_2}{2R^2 - Q_2} \end{cases} \Rightarrow \begin{cases} u_1^1\left(2R^1 - Q_1\right) = e_1 \\ u_2^1\left(2R^1 - Q_2\right) = e_2 \\ u_1^2\left(2R^2 - Q_1\right) = e_1 \\ u_2^2\left(2R^2 - Q_2\right) = e_2 \end{cases} \tag{54}$$

Rewriting this as a set of matrix equations yields

$$\begin{cases} \begin{pmatrix} 1 & u_1^1 \\ 1 & u_1^2 \end{pmatrix} \begin{pmatrix} e_1 \\ Q_1 \end{pmatrix} = \begin{pmatrix} 2u_1^1 R^1 \\ 2u_1^2 R^2 \end{pmatrix} \\ \begin{pmatrix} 1 & u_2^1 \\ 1 & u_2^2 \end{pmatrix} \begin{pmatrix} e_2 \\ Q_2 \end{pmatrix} = \begin{pmatrix} 2u_2^1 R^1 \\ 2u_2^2 R^2 \end{pmatrix} \end{cases} \tag{55}$$

As can be seen, if the inverses of the 2×2-matrices on the left exist, then $\{e_i, Q_i\}_{i\in\{1,2\}}$ can be found in terms of the chosen fixed points and $\left\{R^j\right\}_{j\in\{1,2\}}$. Also, as should be noted, $\left\{R^j\right\}_{j\in\{1,2\}}$ are not known yet, but assume for a moment that they are. For the matrices mentioned to be invertible, the respective determinants must not equal zero. Their determinants are on the form, for $i \in \{1, 2\}$,

$$\begin{vmatrix} 1 & u_i^1 \\ 1 & u_i^2 \end{vmatrix} = u_i^2 - u_i^1 \tag{56}$$

[15]Note that bifurcations can be obtained by varying C: When $C = -\frac{1}{2}S_{jj}$, $R = 0$ so that there is only one fixed point left in the system (that in the origin).

For this to be non-zero $u_i^1 \neq u_i^2 \ \forall i$, i.e. the chosen fixed points *are not allowed to lie along horizontal or vertical lines in the plane to which they are confined.* Assuming this criterion is met, the set of matrix equations becomes

$$\begin{cases} \begin{pmatrix} e_1 \\ Q_1 \end{pmatrix} = \frac{1}{u_1^2-u_1^1} \begin{pmatrix} u_1^2 & -u_1^1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 2u_1^1 R^1 \\ 2u_1^2 R^2 \end{pmatrix} = \frac{1}{u_1^2-u_1^1} \begin{pmatrix} -2u_1^2 u_1^1 \left(R^2 - R^1\right) \\ -2u_1^1 R^1 + 2u_1^2 R^2 \end{pmatrix} \\ \begin{pmatrix} e_2 \\ Q_2 \end{pmatrix} = \frac{1}{u_2^2-u_2^1} \begin{pmatrix} u_2^2 & -u_2^1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 2u_2^1 R^1 \\ 2u_2^2 R^2 \end{pmatrix} = \frac{1}{u_2^2-u_2^1} \begin{pmatrix} -2u_2^2 u_2^1 \left(R^2 - R^1\right) \\ -2u_2^1 R^1 + 2u_2^2 R^2 \end{pmatrix} \end{cases} \tag{57}$$

Now R^1 and R^2 have to be found as well. The equation for $\{R^\alpha\}$ is as before

$$R = \sum_{i=1}^{2} \frac{e_i^2}{2R - Q_i} \tag{58}$$

Using the newly found expressions for $\{e_i, Q_i\}_{i\in\{1,2\}}$ gives these as

$$\begin{cases} R^1 = \left(u_1^1\right)^2 + \left(u_2^1\right)^2 \\ R^2 = \left(u_1^2\right)^2 + \left(u_2^2\right)^2 \end{cases} \tag{59}$$

These two are actually known quantities once the two fixed points are chosen. Now the rest of the $\{R^\alpha\}$ are sought. Using the fixed point relation above gives

$$0 = R\left(2R - Q_1\right)^2 \left(2R - Q_2\right)^2 - e_1^2 \left(2R - Q_2\right)^2 - e_2^2 \left(2R - Q_1\right)^2 \equiv P_5(R) \tag{60}$$

where the polynomial $P_5(R)$ has been defined. As can be seen, $\deg P_5(R) = 5$, but since two roots are already known, R^1 and R^2, the polynomial can be factorized into one of degree three, $P_3(R)$, and one of degree two, $P_2(R)$ (where $P_2(R)$ has solutions R^1 and R^2). This can be written as

$$P_5(R) = P_3(R)P_2(R) = \left(R - R^1\right)\left(R - R^2\right) P_3(R) \tag{61}$$

or

$$\frac{P_5(R)}{\left(R - R^1\right)\left(R - R^2\right)} = P_3(R) \tag{62}$$

For polynomials of degree three, according to the Abel-Ruffini theorem, there exist general expressions for the roots. These are not presented here since they are easily found elsewhere.

It might be good at this point to summarize what has thus far been done:

1. Two fixed points, $\mathbf{u}^1$ and $\mathbf{u}^2$, are chosen.
2. This leads to e_1, e_2, Q_1, Q_2, R^1 and R^2 being found.
3. Using R^1 and R^2, the rest of the R^α can be found, and hence the remaining three fixed points.

3.2.4 A system of two-component vectors: Case (ii)

As was noted earlier, the origin is always a fixed point in this case. Also, whole hyper-spheres of fixed points can be obtained if the matrix elements S_{ii} are chosen such that $S_{11} = S_{22}$. Of course, such systems can be interesting to study, but here the studied case is instead when there exists only one i such that $u_i \neq 0$ and $S_{11} \neq S_{22}$. As was found earlier, this means that there are two fixed points on each coordinate axis as well as the one in the origin. This can be summarized as:

1. The origin $(0, 0)$ is a fixed point.
2. There are four other fixed points in the system given by $\left(\pm\sqrt{-C - \frac{1}{2}S_{11}}, 0\right)$ and $\left(0, \pm\sqrt{-C - \frac{1}{2}S_{22}}\right)$.

If the fixed points are complex with non-zero imaginary part, then they are uninteresting since phase space is real.

Now either C, S_{11} and S_{22} can be chosen to give the four fixed points, or, conversely, the fixed points as well as one of C, S_{11} and S_{22} can be chosen to give the last two values.

3.2.5 A system of two-component vectors: Stabilities, winding numbers and patterns

The analysis presented in this section is applicable to both case (i) and case (ii).

Stability of fixed points

To find the respective stabilities of the fixed points, the eigenvalues of the local[16] Jacobian $\mathbf{J}$ of the mapping at the fixed point must be found (see e.g. the discussion in [1]). The main idea is that the distance between a trajectory and the fixed point in phase space, define it as ϵ, can be written, in obvious notation, as $\epsilon^+ = \mathbf{J}\epsilon$ under the mapping, where the Jacobian then can be diagonalized to yield a relation between trajectory distance and eigenvalues. Since this distance does not take into account higher-order terms in ϵ, this is only true on a *local* (infinitesimal) scale, i.e. once ϵ is not small, non-linear effects have to be considered. The Jacobian for the mapping T from eq. (44) can be written

$$\mathbf{J} = \begin{pmatrix} \left[\nabla_{\mathbf{u}} \otimes (\mathbf{f}(\mathbf{u}) - \mathbf{t})\right]^\top & \left[\nabla_{\mathbf{t}} \otimes (\mathbf{f}(\mathbf{u}) - \mathbf{t})\right]^\top \\ \left[\nabla_{\mathbf{u}} \otimes \mathbf{u}\right]^\top & \left[\nabla_{\mathbf{t}} \otimes \mathbf{u}\right]^\top \end{pmatrix} \tag{63}$$

where $\otimes$ is the usual outer product for vectors[17], and $\nabla_{\mathbf{a}}$, for vector $\mathbf{a} \in \mathbb{R}^2$, is $\nabla_{\mathbf{a}} = (\partial_{a_1}, \partial_{a_2})$. Calculating the easier derivatives gives the Jacobian as

$$\mathbf{J} = \begin{pmatrix} \left[\nabla_{\mathbf{u}} \otimes \mathbf{f}(\mathbf{u})\right]^\top & -\mathbf{1}_2 \\ \mathbf{1}_2 & \mathbf{0}_2 \end{pmatrix} \tag{64}$$

[16] That is, at the fixed point.

[17] For two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^2$, the outer product becomes a 2×2-matrix. In mathematical notation, $\mathbf{a} \otimes \mathbf{b} \in \mathbb{R}^{2\times 2}$

where $\mathbf{1}_2$ and $\mathbf{0}_2$ is the unit matrix and null matrix of size 2×2, respectively. The matrix $[\nabla_{\mathbf{u}} \otimes \mathbf{f}(\mathbf{u})]^\top$ can be written as, for $\mathbf{f}(\mathbf{u}) = (f_1(\mathbf{u}), f_2(\mathbf{u}))$,

$$[\nabla_{\mathbf{u}} \otimes \mathbf{f}(\mathbf{u})]^\top = \begin{pmatrix} \partial_{u_1} f_1 & \partial_{u_2} f_1 \\ \partial_{u_1} f_2 & \partial_{u_2} f_2 \end{pmatrix} \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{65}$$

where a, b, c and d have been defined for simpler upcoming calculations. However, this matrix can be diagonalized such that $[\nabla_{\mathbf{u}} \otimes \mathbf{f}(\mathbf{u})]^\top \to \tilde{\mathbf{f}}(\mathbf{u}) = \mathrm{diag}(\mu_1, \mu_2)$ for eigenvalues μ_1 and μ_2, by similarity-transforming $\mathbf{J}$ using the matrix

$$\mathbf{U} = \begin{pmatrix} \mathbf{T} & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{T} \end{pmatrix} \tag{66}$$

and its inverse

$$\mathbf{U}^{-1} = \begin{pmatrix} \mathbf{T}^{-1} & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{T}^{-1} \end{pmatrix} \tag{67}$$

with a suitable 2×2-matrix $\mathbf{T}$ (for a derivation of the kind of matrix used, see app. B), such that $\mathbf{J} \to \tilde{\mathbf{J}} = \mathbf{U}^{-1}\mathbf{J}\mathbf{U}$. The transformation yields

$$\tilde{\mathbf{J}} = \begin{pmatrix} \mu_1 & 0 & -1 & 0 \\ 0 & \mu_2 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{68}$$

Note that the unit matrices in $\mathbf{J}$ did not change under the transformation, as they, of course, cannot (because it is the same $\mathbf{T}$ along the diagonal in $\mathbf{U}$). Also note that the diagonalization mixes components u_1 and u_2 as well as t_1 and t_2, respectively. Define the new components as $(\tilde{u}_1, \tilde{u}_2, \tilde{t}_1, \tilde{t}_2)$, whose relation to the old components is $(u_1\ u_2\ t_1\ t_2)^\top = \mathbf{U}\,(\tilde{u}_1\ \tilde{u}_2\ \tilde{t}_1\ \tilde{t}_2)^\top$.

This transformed local Jacobian can be written as the sum of the direct products ($\otimes$) between some matrices[18], i.e.

$$\begin{aligned} \tilde{\mathbf{J}} &= \begin{pmatrix} \tilde{\mathbf{f}}(\mathbf{u}) & \mathbf{0}_2 \\ \mathbf{0}_2 & \mathbf{0}_2 \end{pmatrix} + \begin{pmatrix} \mathbf{0}_2 & -\mathbf{1}_2 \\ \mathbf{1}_2 & \mathbf{0}_2 \end{pmatrix} = \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \tilde{\mathbf{f}}(\mathbf{u}) + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \tag{69}$$

Reversing the order of factors in the respective direct products yields the equivalent $\tilde{\mathbf{J}}$ in $(\tilde{u}_1, \tilde{t}_1, \tilde{u}_2, \tilde{t}_2)$-space[19]. Doing this gives

$$\begin{aligned} \tilde{\mathbf{J}} &= \tilde{\mathbf{f}}(\mathbf{u}) \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \\ &= \left(\begin{array}{cc|cc} \mu_1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & \mu_2 & -1 \\ 0 & 0 & 1 & 0 \end{array}\right) \end{aligned} \tag{70}$$

[18] This operator is here defined as, for 2×2-matrices $\mathbf{B}$ and $\mathbf{C}$, $\mathbf{B} \otimes \mathbf{C} \in \mathbb{R}^{4\times 4}$. The matrix on the left, here $\mathbf{B}$, represents the over-all structure of the resulting 4×4-matrix, whereas that on the right, here $\mathbf{C}$, represents the fine-structure. The exact workings of the operation should be obvious from the text.

[19] This is equivalent to reversing the orders of columns two and three as well as rows two and three in $\tilde{\mathbf{J}}$.

where the lines are there to indicate that this is actually a block-diagonal matrix. The eigenvalues $\{\lambda_m\}_{m\in\{1,2,3,4\}}$ to this matrix are therefore easily found: they are just the eigenvalues to the two matrices along the diagonal. Calculating these gives

$$\begin{aligned}\lambda &\in \left\{\frac{\mu_1+\sqrt{\mu_1^2-4}}{2}, \frac{\mu_1-\sqrt{\mu_1^2-4}}{2}, \frac{\mu_2-\sqrt{\mu_2^2-4}}{2}, \frac{\mu_2+\sqrt{\mu_2^2-4}}{2}\right\} \equiv \\ &\equiv \{\lambda_1,\lambda_2,\lambda_3,\lambda_4\} \end{aligned} \tag{71}$$

where $\lambda_{1,2}$ correspond to the upper block, and $\lambda_{3,4}$ to the lower. Now, μ_1 and μ_2 are

$$\{\mu_1,\mu_2\} = \left\{\frac{1}{2}\left(a+d+\sqrt{(a-d)^2+4cb}\right), \frac{1}{2}\left(a+d-\sqrt{(a-d)^2+4cb}\right)\right\} \tag{72}$$

The variables a, b, c and d are given by

$$\begin{aligned}&[\nabla_{\mathbf{u}} \otimes \mathbf{f}(\mathbf{u})]^\top = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \\ = &\frac{1}{\left((u_1)^2+(u_2)^2+C\right)^2}\begin{pmatrix} -2u_1\left(-s_{11}u_1+e_1\right)-s_{11}\left((u_1)^2+(u_2)^2+C\right) & 0 \\ -2u_1\left(-s_{22}u_2+e_2\right) & 0 \end{pmatrix} + \\ + &\frac{1}{\left((u_1)^2+(u_2)^2+C\right)^2}\begin{pmatrix} 0 & -2u_2\left(-s_{11}u_1+e_1\right) \\ 0 & -2u_2\left(-s_{22}u_2+e_2\right)-s_{22}\left((u_1)^2+(u_2)^2+C\right) \end{pmatrix}\end{aligned}$$

It is easy to check that the product of all the eigenvalues equals one, but it is also easy to see that $\lambda_1\lambda_2 = \lambda_3\lambda_4 = 1$, i.e., the corresponding eigenvectors pairwise define orthogonal planes[20] in phase space (which together span the whole space) where area is preserved under the mapping. This could already be noted in the block-diagonal matrix above, since each block on the diagonal has unit determinant. As can be seen, there is a clear C-dependence[21] (C from eq. (46)) in $\{\lambda_m\}$, so that the respective stabilities also depend on C. It should be noted that $\lambda \in \mathbb{C}$, but fixed point stabilities are fundamentally different if $\mathrm{Im}\,\lambda = 0$. The differences can be summarized according to (where x is the spatial dimension of the system):

1. If $\mathrm{Im}\,\lambda \neq 0\ \forall\lambda$, the fixed point is *elliptic*, and oscillating behaviour in x is present. These fixed points are the interesting ones since it is around such (at infinitesimal distances) that (quasi-)periodic patterns can arise [3]. From eq. (71) it can be seen that μ_1 and μ_2 must fulfill $\mu_1,\mu_2 \in (-2,2)$ for a fixed point to be elliptic.

2. If $\exists\lambda : \mathrm{Im}\,\lambda = 0$, the fixed point is partly *hyperbolic*, i.e., it has exponential behaviour. As an effect, the corresponding pattern almost always will have ever-(in/de)creasing amplitude [3]. Because of this, these are not interesting in the current analysis. Eq. (71) states that $\mu_1 \vee \mu_2 \notin (-2,2)$ for a fixed point to be hyperbolic.

[20] These planes are the $(\tilde{u}_1,\tilde{t}_1)$-plane and the $(\tilde{u}_2,\tilde{t}_2)$-plane, respectively.

[21] This dependence could also be on e.g. S_{11} or S_{22}, since there is only one free parameter left once the two fixed points have been chosen. Note that once the parameter is chosen, all other parameters are known. Here, C is considered the free parameter. The relation between S_{ii} ($i \in \{1,2\}$) and C is, as was mentioned earlier, $Q_i = -2C - S_{ii}$.

It should be noted that the oscillations occur in *lattice space*: the analysis says nothing about whether or not the patterns are stable in time under the RD-dynamics (or, for that matter, under some other dynamics, since the static case studied is not uniquely defined by the RD-dynamics).

Now that the stabilities have been analyzed, the possible patterns remain to be studied.

The winding number and its connection to patterns

To start investigating the patterns, it should be noted that since, for the elliptic fixed points, the eigenvalues $\mu_i \in (-2, 2)\ \forall i \in \{1, 2\}$, each μ_i can be seen as twice a cosine-function, or, put equivalently, $\frac{\mu_i}{2} = \cos(2\pi w_i)$, for some number w_i. This number, w_i, is usually referred to as the *winding number*, and has the following properties [3]:

1. If w_i is rational, i.e. $w_i = p/q$ for relatively prime integers p, q such that $0 \leq p < q$, then the trajectories at infinitesimal distances from the fixed point in the corresponding phase space plane are *periodic*[22] of period q.
2. If w_i is irrational, then the trajectories at infinitesimal distances from the fixed point in the corresponding phase space plane are *quasi-periodic*[23].

The winding number can in terms of μ_i be rewritten as

$$w_i = \frac{1}{2\pi} \arccos\left(\frac{\mu_i}{2}\right) \in \left[0,\ \frac{1}{2}\right] \tag{73}$$

Since there is a dependence on C in μ_i, so there is in w_i. Because of this, C can be chosen in such a way that w_i becomes rational or irrational. Sometimes it is even possible to choose C such that both w_i's are of the same kind.

As was stated above, the winding numbers correspond to periodic or quasi-periodic motion in the planes spanning the local phase space around a point, so that the respective patterns there should have the corresponding characteristics. It should be noted that the winding number is defined for a trajectory starting at an *infinitesimal* distance from a point, so that it for any perturbation not infinitesimal is just an approximation. Hence, in the respective planes, the characteristics of the patterns connected to the winding number should only be visible for small enough initial perturbations. Also, at distances not small enough, the planes are bent into more complicated surfaces in the four-dimensional space.

Now, the sought patterns in the quantities (u_1, u_2, t_1, t_2) must show characteristics that are combinations of those for the patterns in $(\tilde{u}_1, \tilde{t}_1)$ and $(\tilde{u}_2, \tilde{t}_2)$ respectively. E.g., a sought pattern might have an overall structure like a regular sine-wave, but with tiny ripples along the wave itself (so that the sought pattern is a combination of two different patterns: one for each plane). Therefore, the sought patterns in (u_1, u_2, t_1, t_2) are *quasi-periodic*, i.e. they are combinations of patterns that themselves have oscillating characteristics. However, non-linear effects can affect this behaviour.

[22] The interpretation of this in two-dimensional phase space is easy: q is the number of iterations needed in the mapping to return to the initial value, and p is the number of times the "centre" of the structure is rotated around.

[23] Comparing with the interpretation of the periodic case, quasi-periodicity means that a series of iterations never quite returns to its initial value.

To conclude:

1. If the mapping in eq. (44) is initialized with perturbations in only one of the planes[24], it should for small enough such perturbations be found that the patterns show approximately the correct characteristics (i.e. the characteristics connected to the winding number for the plane in which initial perturbations were used).
2. If small enough initial perturbations are allowed in both local planes, then the resulting pattern should have characteristics that are combinations of the two local planes' respective characteristics.

This is investigated in sec. 4.1.1.

3.2.6 A system of two-component vectors: The conserved quantity and the local planes in phase space

The structure of the conserved quantity $H(\mathbf{u}, \mathbf{v})$ in eq. (47), which in turn is connected to the function $\mathbf{f}(\mathbf{u})$ in eq. (45), is the same for both case (i) and case (ii) (the only difference is the presence of $\mathbf{e}$ in H). Because of this, the following analysis can be held at a general level. For simplicity, the conserved quantity is here referred to as the energy in the system.

As was discussed in sec. 3.2.5, around each fixed point there exist two local orthogonal planes, in which the dynamics is linearized, spanning phase space. It should then be possible to write the energy in local coordinates as a sum of contributions: one for each plane and also one for the higher-order non-linearity (the last one should be small for small enough initial perturbations from the fixed point). It can be interesting to see how the energy is distributed between the two planes and the non-linear term as perturbations are varied in size.

To investigate this, translate $\mathbf{u}$ to a fixed point $\mathbf{u}^*$ so that $\mathbf{u} \longrightarrow \mathbf{u}^* + \mathbf{d}$ where $\mathbf{d}$ is the deviation from the origin in the new space. Of course, this changes the recursion $\mathbf{u}^+ + \mathbf{u}^- = \mathbf{f}(\mathbf{u})$ such that

$$\mathbf{d}^+ + \mathbf{d}^- = \mathbf{f}\left(\mathbf{u}^* + \mathbf{d}\right) - 2\mathbf{u}^* \equiv \tilde{\mathbf{f}}(\mathbf{d}) \tag{74}$$

where $\tilde{\mathbf{f}}(\mathbf{d})$ has been defined for convenience. As can be seen, this is of the same form as the recursion was before the translation. Simplifying $\tilde{\mathbf{f}}\left(\mathbf{d}\right)$ by using the fixed point relation in eq. (50) and letting $\mathbf{u}^*$ be written as $\mathbf{u}$ for convenience gives

$$\tilde{\mathbf{f}}\left(\mathbf{d}\right) = \frac{-2\mathbf{u}\,\mathbf{d}^\top\mathbf{d} + \left(-\mathbf{S} - 4\mathbf{F}\right)\mathbf{d}}{\mathbf{d}^\top\mathbf{d} + 2\mathbf{u}^\top\mathbf{d} + \mathbf{u}^\top\mathbf{u} + C} \tag{75}$$

where the matrix

$$\mathbf{F} \equiv \mathbf{u}\mathbf{u}^\top = \begin{pmatrix} a^2 & ab \\ ab & b^2 \end{pmatrix} \tag{76}$$

[24]Choosing perturbations in (u_1, u_2, t_1, t_2)-space such that only one of the planes contains perturbations is easy: the perturbations in (u_1, u_2, t_1, t_2)-space, $\delta \equiv (\delta u_1, \delta u_2, \delta t_1, \delta t_2)$, are related to those in $(\tilde{u}_1, \tilde{u}_2, \tilde{t}_1, \tilde{t}_2)$-space, $\tilde{\delta} \equiv (\delta\tilde{u}_1, \delta\tilde{u}_2, \delta\tilde{t}_1, \delta\tilde{t}_2)$, by $\delta = \mathbf{U}\tilde{\delta}$, where $\mathbf{U}$ is the transformation matrix from eq. (66).

has been defined for fixed point components a and b, where $\mathbf{u} = (a, b)$. Locally $\tilde{\mathbf{f}}(\mathbf{d})$ becomes linear,

$$\tilde{\mathbf{f}}\,(\mathbf{d}) \sim \frac{(-\mathbf{S} - 4\mathbf{F})\,\mathbf{d}}{\mathbf{u}^2 + C} \tag{77}$$

The translation, of course, also affects the energy function. Define the local energy as[25] $\tilde{H}(\mathbf{d}, \mathbf{g})$, where $\mathbf{g} = \mathbf{v} - \mathbf{v}^*$ for vector $\mathbf{v}$ and fixed point $\mathbf{v}^*$ in the original space. The exact expression for this translated energy is here left out.

As can be noted in the exact expression for $\tilde{\mathbf{f}}(\mathbf{d})$, the matrix $\mathbf{M} \equiv -\mathbf{S} - 4\mathbf{F}$ is not necessarily diagonal, but can be made so by similarity-transforming it with a suitable orthogonal matrix $\mathbf{T}$ (for an example of how to diagonalize a 2×2-matrix see app. B). All vectors and other matrices in the space are thus also transformed, so that

$$\begin{cases} \mathbf{u} \longrightarrow \mathbf{T}^\top \mathbf{u} \\ \mathbf{S} \longrightarrow \mathbf{T}^\top \mathbf{S} \mathbf{T} \\ \mathbf{d} \longrightarrow \mathbf{z} \end{cases} \tag{78}$$

The transformed version of $\tilde{\mathbf{f}}(\mathbf{d})$, $\hat{\mathbf{f}}(\mathbf{z})$, say, becomes

$$\hat{\mathbf{f}}(\mathbf{z}) = \frac{-2\,\mathbf{T}^{-1}\mathbf{u}\,\mathbf{z}^\top \mathbf{z} + \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \mathbf{z}}{\mathbf{z}^\top \mathbf{z} + 2\mathbf{u}^\top \mathbf{T}\,\mathbf{z} + \mathbf{u}^\top \mathbf{u} + C} \tag{79}$$

for eigenvalues σ_1 and σ_2 of $\mathbf{M}$. Locally this function becomes linear,

$$\hat{\mathbf{f}}(\mathbf{z}) \sim \frac{1}{\mathbf{u}^2 + C} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \mathbf{z} \tag{80}$$

Comparing eqs. (40) and (79), and then using eq. (42), gives the new local energy $\hat{H}(\mathbf{z}, \mathbf{w})$ (with the same properties as $\tilde{H}(\mathbf{d}, \mathbf{g})$) as

$$\begin{aligned} \hat{H}(\mathbf{z}, \mathbf{w}) &= \mathbf{z}^2\mathbf{w}^2 + 2\,\mathbf{z}^2\mathbf{u}^\top \mathbf{T}\,\mathbf{w} + 2\,\mathbf{w}^2\mathbf{u}^\top \mathbf{T}\,\mathbf{z} + \\ &+ \mathbf{z}^2\left[\mathbf{u}^2 + C\right] + \mathbf{w}^2\left[\mathbf{u}^2 + C\right] \\ &- \mathbf{z}^\top \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \mathbf{w} \end{aligned} \tag{81}$$

for vectors $\mathbf{z} = (z_1, z_2)$ and $\mathbf{w} = (w_1, w_2)$ representing the perturbations from the origin in the respective directions in the new space. The two orthogonal local planes are the (z_1, w_1)-plane and the (z_2, w_2)-plane, respectively. The three first terms are the higher-order non-linear ones, and of the three remaining there is only one that couples the different components: the last one. Because of the structure of the matrix there, the term is such that z_1 only couples to w_1 and conversely for z_2 and w_2, which in turn means that $\hat{H}(\mathbf{z}, \mathbf{w})$ can be written as the sum of three contributions: one quadratic term for the (z_1, w_1)-plane, another quadratic for the (z_2, w_2)-plane, and one for the higher order non-linear

[25] This local energy, since the total energy in the system is conserved, is equal to $H(\mathbf{u}^* + \mathbf{d}, \mathbf{v}^* + \mathbf{g}) - H(\mathbf{u}^*, \mathbf{v}^*)$, for fixed points $\mathbf{u}^*$ and $\mathbf{v}^*$.

terms. Define these as $\hat{H}_1$, $\hat{H}_2$ and $\hat{H}_3$, respectively:

$$\begin{cases} \hat{H}_1 = \left(z_1^2 + w_1^2\right)\left(\mathbf{u}^2 + C\right) - \sigma_1 z_1 w_1 \\ \hat{H}_2 = \left(z_2^2 + w_2^2\right)\left(\mathbf{u}^2 + C\right) - \sigma_2 z_2 w_2 \\ \hat{H}_3 = \mathbf{z}^2\mathbf{w}^2 + 2\,\mathbf{z}^2\mathbf{u}^\top\mathbf{T}\,\mathbf{w} + 2\,\mathbf{w}^2\mathbf{u}^\top\mathbf{T}\,\mathbf{z} \end{cases} \tag{82}$$

Therefore, $\hat{H}(\mathbf{z},\mathbf{w}) = \hat{H}_1 + \hat{H}_2 + \hat{H}_3$. As can be seen, if $\left|\frac{\sigma_i}{\mathbf{u}^2+C}\right| \leq 2$ for $i \in \{1,2\}$, then $\hat{H}_i$ is positive-definite.

The distribution of energy along the lattice , i.e. the distribution of $\hat{H}_1$, $\hat{H}_2$ and $\hat{H}_3$, for fixed points can now be investigated by plotting the three functions for different initial perturbations in the mapping from eq. (44) (with the function $\mathbf{f}(\mathbf{u})$ as in eq. (79)). The fixed points can be as in case (i) or as in case (ii). The following behaviour is expected:

1. For elliptic fixed points the energy between the two planes is expected to oscillate (the higher-order contribution should as well). Such behaviour is analogous to that of non-linearly coupled pendulums.
2. For hyperbolic fixed points the local energy is expected to be very sensitive, i.e. $\mathbf{z}$ and $\mathbf{w}$ are expected to "blow up" even for small perturbations.

This is studied in sec. 4.1.2.

The transformed energy for the N-species case

Eq. (42) is easily generalized to the N-species case: $\mathbf{F}$ is directly generalized so all that has to be done is to diagonalize $\mathbf{M} = -\mathbf{S} - 4\,\mathbf{F}$ with orthogonal $N \times N$-matrix $\mathbf{T}$, so that $\mathbf{M} \to \hat{\mathbf{M}} \equiv \mathrm{diag}\,(\sigma_1, \ldots, \sigma_N)$. The result is

$$\begin{aligned} \hat{H}(\mathbf{z},\mathbf{w}) &= \mathbf{z}^2\mathbf{w}^2 + 2\,\mathbf{z}^2\mathbf{u}^\top\mathbf{T}\,\mathbf{w} + 2\,\mathbf{w}^2\mathbf{u}^\top\mathbf{T}\,\mathbf{z} + \\ &+ \mathbf{z}^2\left[\mathbf{u}^2 + C\right] + \mathbf{w}^2\left[\mathbf{u}^2 + C\right] \\ &- \mathbf{z}^\top\hat{\mathbf{M}}\,\mathbf{w} \end{aligned} \tag{83}$$

As can be seen, this expression can be written as a sum of contributions just as before: $\hat{H}(\mathbf{z},\mathbf{w}) = \sum_{i=1}^{N+1}\hat{H}_i$, where $\hat{H}_{N+1}$ is the higher-order non-linear term and $\hat{H}_i$ is a quadratic term for the plane (z_i, w_i) for all $1 \leq i \leq N$. However, this is not further investigated in this report.

4 Results and discussion

In this section examples connected to the theoretical results in sec. 3 are presented. At the end of the section general results are discussed.

4.1 Examples

The examples are presented in the different subsections. Each of these is referred to from the corresponding place in sec. 3.

4.1.1 Quasi-periodic patterns

In this example case (i) is studied (see sec. 3.2.3):

Choosing $\mathbf{u}^1 \equiv (u_1^1, u_2^1) = (1/2, 1/2)$ and $\mathbf{u}^2 \equiv (u_1^2, u_2^2) = (-1, 1)$ (which are allowed since they do not lie on the same horizontal or vertical line) gives the needed parameter values, see table 1. Knowing these values yields the three remaining fixed points easily. For convenience, these are presented as in table 2 below (in the same notation as above).

Table 1: Parameter values

	Parameter values
e_1	-1
e_2	-3
Q_1	3
Q_2	7
R^1	$1/2$
R^2	2
R^3	$5/2$
R^4	$(5+2\sqrt{3})/2$
R^5	$(5-2\sqrt{3})/2$

Table 2: Fixed points

	Coordinates
$\mathbf{u}^1$	$(1/2, 1/2)$
$\mathbf{u}^2$	$(-1, 1)$
$\mathbf{u}^3$	$(-1/2, 3/2)$
$\mathbf{u}^4$	$\left(\frac{-1}{2+2\sqrt{3}}, \frac{-3}{-2+2\sqrt{3}}\right)$
$\mathbf{u}^5$	$\left(\frac{-1}{2-2\sqrt{3}}, \frac{-3}{-2-2\sqrt{3}}\right)$

The stabilities of these fixed points can be found by looking at the dependence on C for μ_1 and μ_2. The typical behaviour of μ_1 and μ_2 for the fixed points is shown in figs. 2 and 3. As can be seen in fig. 2, there exists no C such that $\mathbf{u}^5$ or $\mathbf{u}^2$ becomes elliptic: one of the eigenvalues μ is always outside the interval $[-2, 2]$. Therefore, these two fixed points are uninteresting when it comes to investigating the patterns. The other three fixed points can be elliptic, as is seen in fig. 3, but it is not possible to have all three of them as such for a chosen C (this is not shown in the fig. due to the inconvenience of having several relatively similar functions in the same graph).

Now, choosing $C = \left(\frac{5}{2}\sqrt{3} - \sqrt{13}\right)\left(\sqrt{3}+2\right)$ gives winding numbers and eigenvalues as in table 3. As can be seen, for this C the elliptic fixed points are $\mathbf{u}^3$ and $\mathbf{u}^4$. Also, the winding numbers are well-approximated by simple rational numbers for $\mathbf{u}^3$ (which can be seen from a continued fraction expansion). For fixed point $\mathbf{u}^3$ it can now be investigated whether or not quasi-periodic patterns can be obtained. This is shown in figs.[26] 4–6. *As can be seen, quasi-periodic patterns with specific characteristics can be found just as the theory predicts.*

[26] All of the figures were created by choosing perturbations δ_1 and δ_2 such that the mapping in eq. (44) was initialized with perturbation δ_1 for both components in the (u_1, t_1)-plane, and perturbation δ_2 for the components in the (u_2, t_2)-plane. The initial point (u_1, u_2, t_1, t_2) was the fixed point $(\mathbf{u}^3, \mathbf{u}^3)$.

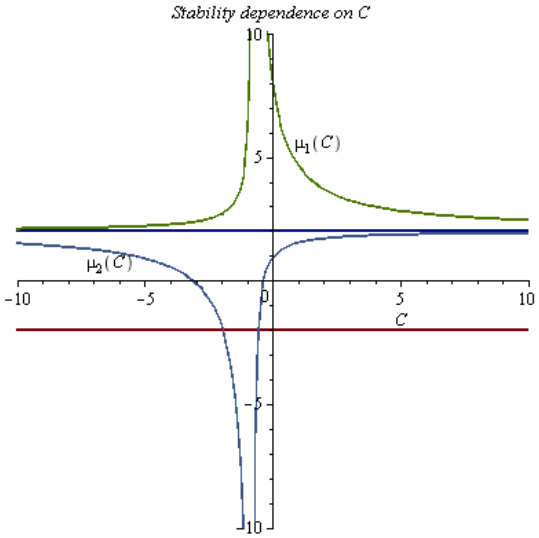

Figure 2: Stability dependence on C for $\mathbf{u}^5$: The eigenvalues μ_1 and μ_2 are here plotted against the parameter C. As can be seen, there does not exist any C value such that the fixed point is elliptic (i.e., where $\mu_1, \mu_2 \in (-2, 2)$). Fixed point $\mathbf{u}^2$ has a similar behaviour.

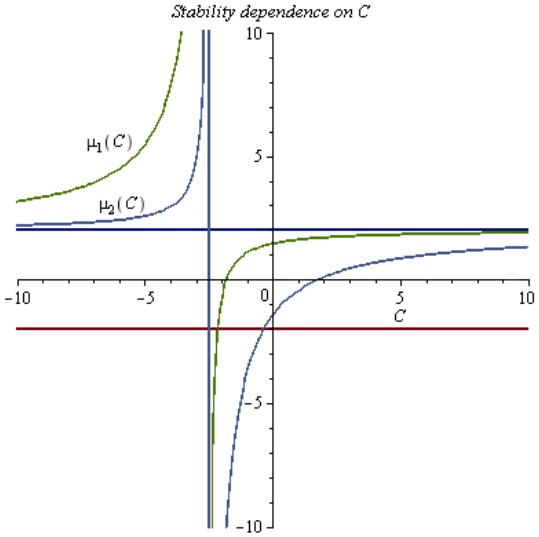

Figure 3: Stability dependence on C for $\mathbf{u}^3$: The eigenvalues μ_1 and μ_2 are here plotted against the parameter C. As can be seen, there exist several C values for which the fixed point is elliptic (i.e., where $\mu_1, \mu_2 \in (-2, 2)$). Fixed points $\mathbf{u}^1$ and $\mathbf{u}^4$ have a similar behaviour.

Table 3: Winding numbers and eigenvalues

	μ_1	μ_2	w_1	w_2
$\mathbf{u}^1$	3.634150166	2.238419296	Hyp.	Hyp.
$\mathbf{u}^2$	2.312943860	0.4115875560	Hyp.	0.2170111944
$\mathbf{u}^3$	1.732050808	0.3464071005	$0.08333333330 \approx 1/12$	$0.2222940756 \approx 2/9$
$\mathbf{u}^4$	1.218191745	-0.6575954013	0.1457662296	0.3033217142
$\mathbf{u}^5$	3.353471734	1.757211562	Hyp.	0.07923712710

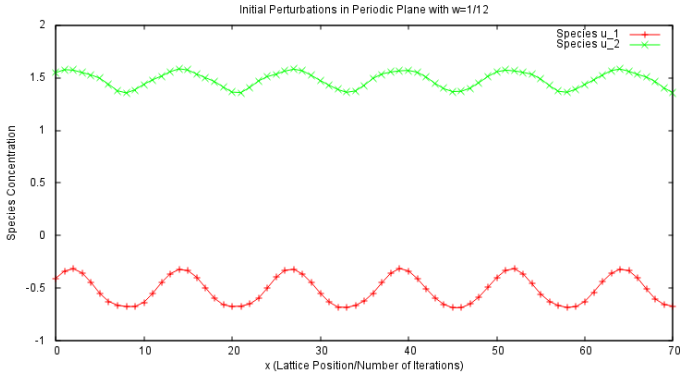

Figure 4: Here u_1 and u_2 are plotted against the number or iterations (i.e., lattice position) for fixed point $\mathbf{u}^3$ where perturbations were used only in the local plane where $w_1 = 1/12$. As can be seen, the patterns appear roughly periodic with period 12, which agrees with the predictions. The initial perturbations for u_1 and u_2 were $\sim 5 \cdot 10^{-2}$.

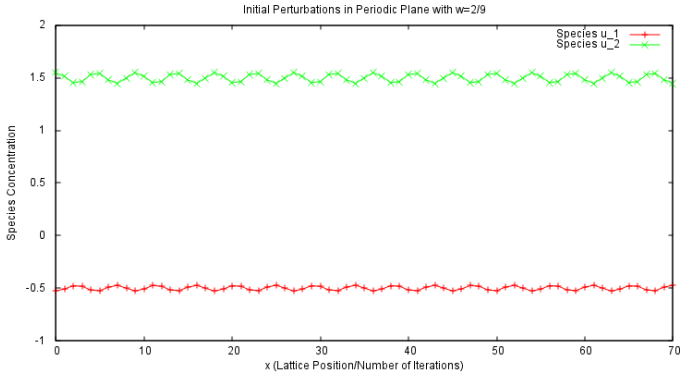

Figure 5: Here u_1 and u_2 are plotted against the number or iterations (i.e., lattice position) for fixed point $\mathbf{u}^3$ where perturbations were used only in the local plane where $w_2 = 2/9$. As can be seen, the patterns appear roughly periodic with period 9, which agrees with the predictions. The initial perturbations for u_1 and u_2 were $\sim 5 \cdot 10^{-2}$.

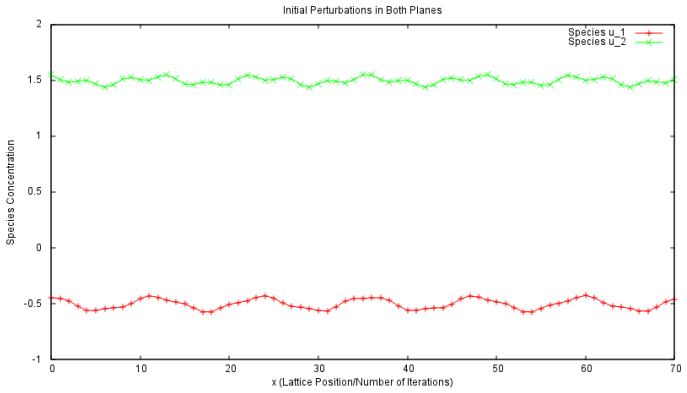

Figure 6: Here u_1 and u_2 are plotted against the number or iterations (i.e., lattice position) for fixed point $\mathbf{u}^3$ where perturbations were used in both local planes. As can be seen, each pattern appears to be a combination of independent oscillations, which then classifies the patterns as quasi-periodic. The initial perturbations for u_1 and u_2 were $\sim 5 \cdot 10^{-2}$.

4.1.2 Energy in the local planes and non-linear effects

Case (i)

Finding fixed points as in sec. 3.2.3 gives parameter values and fixed points as in tables 4 and 5. Note that in table 5 the stabilities have also been included for $C = 2\left(5\sqrt{3} - 2\sqrt{13}\right)\left(\sqrt{3}+2\right)$. The energy distribution for elliptic fixed point

Table 4: Parameter values

	Parameter values
e_1	-24
e_2	-8
Q_1	28
Q_2	12
R^1	2
R^2	10
R^3	$10+4\sqrt{3}$
R^4	$10-4\sqrt{3}$
R^5	8

Table 5: Fixed points

	Coordinates	Stabilities
$\mathbf{u}^1$	$(1,1)$	Hyp.
$\mathbf{u}^2$	$(3,-1)$	Ell.
$\mathbf{u}^3$	$\left(\frac{-3}{-1+\sqrt{3}}, \frac{-1}{1+\sqrt{3}}\right)$	Ell.
$\mathbf{u}^4$	$\left(\frac{3}{1+\sqrt{3}}, \frac{-1}{1-\sqrt{3}}\right)$	Hyp.
$\mathbf{u}^5$	$(2,-2)$	Ell.

$\mathbf{u}^2$ is shown for different perturbations in figs. 7 and 8. Also, the local energy distribution for hyperbolic fixed point $\mathbf{u}^1$ is shown in fig. 9.

For elliptic fixed point $\mathbf{u}^2$, $\sigma_1 = 2C + \sqrt{208}$ and $\sigma_2 = 2C - \sqrt{208}$, so that the two local quadratic energies become ($\hat{H}_3$ is left out due to its complexity)

$$\begin{cases} \hat{H}_1 = (10+C)\left(z_1^2 + w_1^2 - \frac{2C+\sqrt{208}}{10+C} z_1 w_1\right) \\ \hat{H}_2 = (10+C)\left(z_2^2 + w_2^2 - \frac{2C-\sqrt{208}}{10+C} z_2 w_2\right) \end{cases} \tag{84}$$

where the exact expression for C has been left out for simplicity. Numerically $\left|\frac{2C\pm\sqrt{208}}{10+C}\right| \leq 2$ so that $\hat{H}_1$ and $\hat{H}_2$ must be positive-definite functions.

For the hyperbolic fixed point $\mathbf{u}^1$, $\sigma_1 = 2C+16+\sqrt{80}$ and $\sigma_2 = 2C+16-\sqrt{80}$, so that the two local quadratic energies here become ($\hat{H}_3$ is left out due to its complexity)

$$\begin{cases} \hat{H}_1 = (2+C)\left(z_1^2 + w_1^2 - \frac{2C+16+\sqrt{80}}{2+C} z_1 w_1\right) \\ \hat{H}_2 = (2+C)\left(z_2^2 + w_2^2 - \frac{2C+16-\sqrt{80}}{2+C} z_2 w_2\right) \end{cases} \tag{85}$$

where the exact expression for C has been left out for simplicity. Numerically $\left|\frac{2C+16\pm\sqrt{80}}{2+C}\right| \geq 2$ so that $\hat{H}_1$ and $\hat{H}_2$ *cannot* be positive-definite functions.

Fig. 8 clearly shows that the two partial energies (of the local planes) behave similar to the energies of two non-linearly coupled pendulums, i.e. as was expected. Also, the simulation in fig. 9 clearly shows the unstable nature of hyperbolic fixed points. Once again the system was found to behave as expected. The respective characteristics of H_1 and H_2 agree with the theory in all simulations.

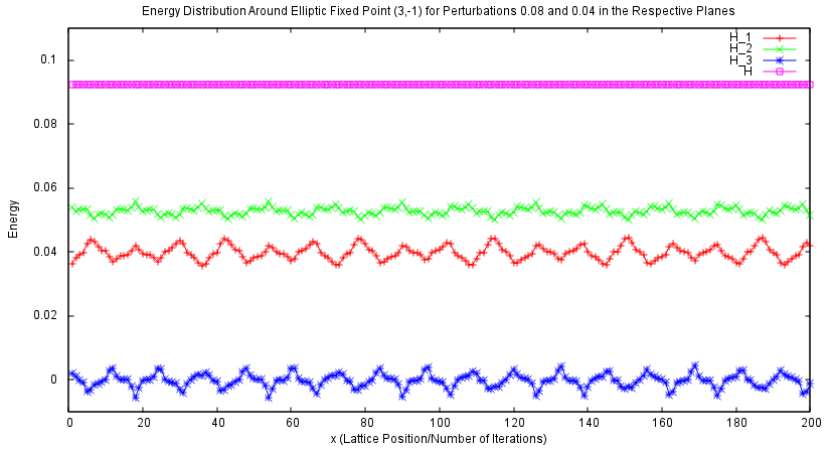

Figure 7: Here the local partial energies $\hat{H}_1$, $\hat{H}_2$, $\hat{H}_3$ and $\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3$ are plotted against lattice position (number of iterations) for elliptic fixed point $\mathbf{u}^2$ using initial perturbation 0.08 for both components in the (z_1, w_1)-plane and initial perturbation 0.04 for both components in the (z_2, w_2)-plane. As can be seen, the total energy H is conserved, and the different contributions oscillate. As expected, $\hat{H}_1$ and $\hat{H}_2$ are positive-definite.

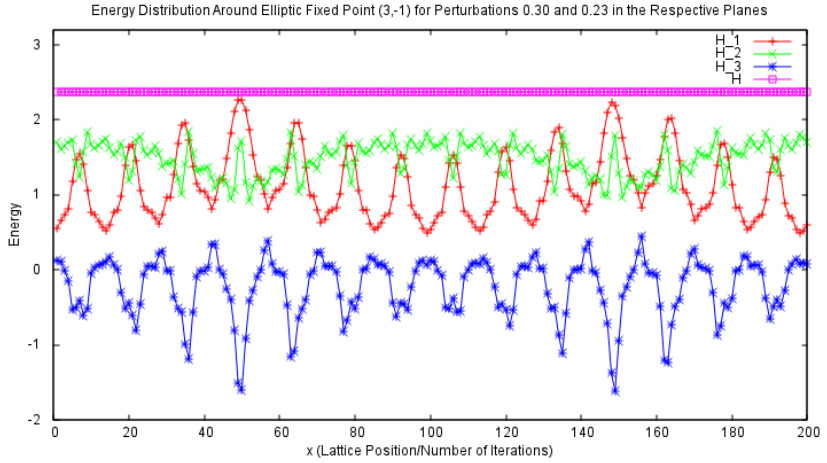

Figure 8: Here the local partial energies $\hat{H}_1$, $\hat{H}_2$, $\hat{H}_3$ and $\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3$ are plotted against lattice position (number of iterations) for elliptic fixed point $\mathbf{u}^2$ using initial perturbation 0.30 for both components in the (z_1, w_1)-plane and initial perturbation 0.23 for both components in the (z_2, w_2)-plane. As can be seen, the total energy $\hat{H}$ is conserved, and the different contributions oscillate. Note that as the mean value of $\hat{H}_1$ goes up, that of $\hat{H}_2$ goes down (and conversely), all the while $\hat{H}_3$ oscillates. When looking at just the two planes' energies, the situation is quite similar to that of coupled pendulums. Also, as expected, $\hat{H}_1$ and $\hat{H}_2$ are positive-definite.

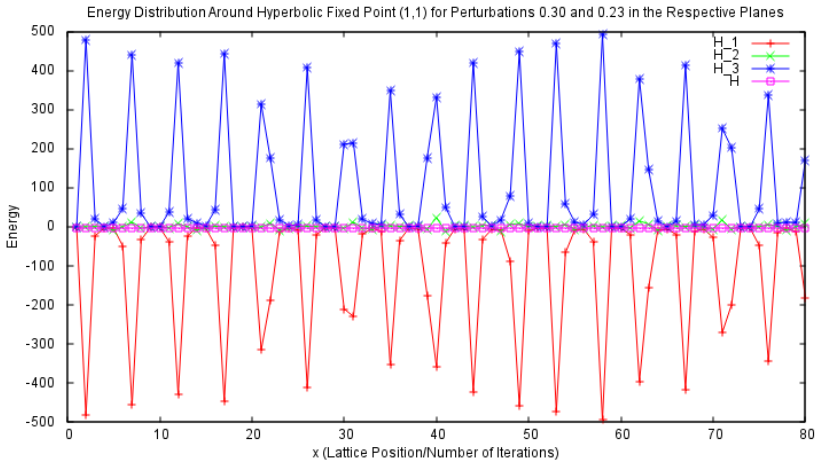

Figure 9: Here the local partial energies $\hat{H}_1$, $\hat{H}_2$, $\hat{H}_3$ and $\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3$ are plotted against lattice position (number of iterations) for hyperbolic fixed point $\mathbf{u}^1$ using initial perturbation 0.30 for both components in the (z_1, w_1)-plane and initial perturbation 0.23 for both components in the (z_2, w_2)-plane. As can be seen, the total energy $\hat{H}$ is conserved (it is roughly -2), and the different contributions oscillate. When comparing the magnitude of the energy with that in fig. 8, it is seen that it here has "blown up" (both systems have the same, for the planes, respective initial perturbations). As expected, $\hat{H}_1$ and $\hat{H}_2$ are not positive-definite functions.

Case (ii)

Now, according to sec. 3.2.4 the fixed points can be chosen as $(\pm 2, 0)$ and $(0, \pm 1)$. For $C = 1$ this gives parameter values and stabilities as in tables 6 and 7. The energy distribution for fixed point $\mathbf{u}^2$ is shown in fig. 10. As can be seen when compared to figs. 7 and 8, the analysis works just as well for fixed points determined from case (ii).

For elliptic fixed point $\mathbf{u}^2$, $\sigma_1 = -6$ and $\sigma_2 = 4$, so that the two local quadratic energies become ($\hat{H}_3$ is left out due to its complexity)

$$\begin{cases} \hat{H}_1 = 5\left(z_1^2 + w_1^2 + \frac{6}{5} z_1 w_1\right) \\ \\ \hat{H}_2 = (10 + C)\left(z_2^2 + w_2^2 - \frac{4}{5} z_2 w_2\right) \end{cases} \tag{86}$$

As can be seen, these must be positive-definite functions. Fig. 10 shows that the analysis works for fixed points of case (ii) as well.

Table 6: Parameter values

	Parameter values
S_{11}	-10
S_{22}	-4

Table 7: Fixed points

	Coordinates	Stabilities
$\mathbf{u}^1$	$(0, 0)$	Hyp.
$\mathbf{u}^2$	$(2, 0)$	Ell.
$\mathbf{u}^3$	$(-2, 0)$	Ell.
$\mathbf{u}^4$	$(0, 1)$	Hyp.
$\mathbf{u}^5$	$(0, -1)$	Hyp.

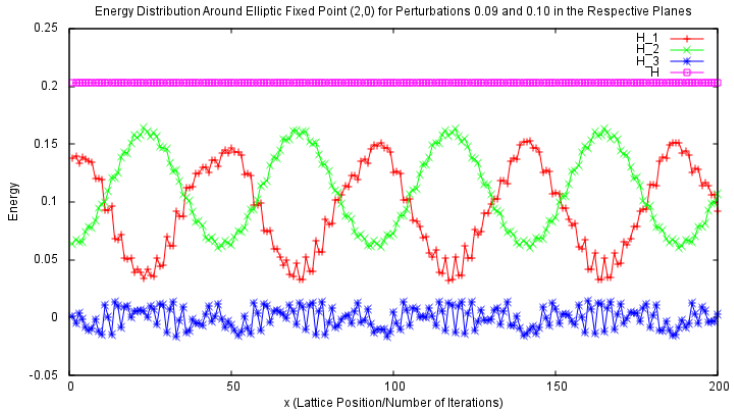

Figure 10: Here the local partial energies $\hat{H}_1$, $\hat{H}_2$, $\hat{H}_3$ and $\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3$ are plotted against lattice position (number of iterations) for elliptic fixed point $\mathbf{u}^2$ using initial perturbation 0.09 in the (z_1, w_1)-plane and initial perturbation 0.10 in the (z_2, w_2)-plane. As can be seen, the total energy $\hat{H}$ is conserved, and the different contributions oscillate just as they do in figs. 7 and 8. Also, $\hat{H}_1$ and $\hat{H}_2$ are positive-definite, as they should. This picture shows that the analysis for case (ii) works as well.

4.2 General results and discussion

The general results can be concluded and discussed as:

1. *Generalizing the known class of conservative maps for the one-dimensional system of one species to higher dimensionality of independent variables is impossible.*

   That it is impossible to generalize the method is interesting in itself, but since it is unclear whether or not there exists only one kind of $f(u)$ that gives a conserved quantity in the one-dimensional one-species case or not, it is not possible to say whether or not further investigations of these systems are unnecessary.

2. *For all mappings as in eq. (44), there exists at least one conserved quantity on the form of eq. (47) for each function on the form of eq. (45).*

   The existence of this conserved quantity restricts the trajectories in phase space to lie on $(2N-1)$-dimensional hypersurfaces. A system with d degrees of freedom is called integrable if there are d independent conserved quantities, and unless all of these exist there is a possibility of chaos in the system [1]. Therefore, it would have been interesting to try to find a parametrization of the $(2N-1)$-dimensional hypersurface defined by the conserved quantity found, and investigate whether or not the trajectories embedded there are chaotic or not. If they are, then the system is not integrable and the found quasi-periodic patterns are not truly quasi-periodic[27].

3. *For these mappings there are fixed points satisfying eq. (50) which in the $(N=2)$-case can be found as in sec. 3.2.3 or sec. 3.2.4, depending on what system is studied. These fixed points can be either hyperbolic or elliptic, something which can be decided using the tools developed in sec. 3.2.5.*

   These tools only apply to the $(N=2)$-case, but it should be possible to generalize these to a higher number of vector components.

4. *Around the elliptic fixed points for the $(N=2)$-case quasi-periodic patterns along the lattice can be found near elliptic fixed points. These quasi-periodic patterns are combinations of the oscillations in the two local (around the fixed point) planes spanning the four-dimensional phase space (Sec. 4.1.1).*

   The existence of quasi-periodic patterns for the $(N=2)$-case is of course intriguing, but as was mentioned in sec. 3.2.5 their stability in time is unclear. The reason for this is that the actual RD-dynamics were not studied, only the static case was. Also, since the static EoM investigated could result from some dynamics different from the RD-dynamics, it might be that the patterns are stable under such instead/as well. It would also be interesting to see whether or not any real biological systems could be described by the investigated kinds of systems.

[27] This since there does not exist a full set of action and angle variables (see e.g. [1]).

5. *The conserved quantity can be investigated in a coordinate system around any point (where the only difference to the actual energy is an additive constant), so that it obtains the form of eq. (83). For the* $(N = 2)$*-case, the distribution of energy between the two planes around an elliptic fixed point resembles that of two non-linearly coupled pendulums (Sec. 4.1.2).*

   This behaviour of the distribution of local energy should generalize, for the N-species case (see eq. (83)), such that the energy distribution resembles that of N non-linearly coupled pendulums. To investigate this, a method of finding fixed points for an N-dimensional system would have to be found.

5 Summary

The formation of quasi-periodic patterns in discrete reaction-diffusion-systems of different dimensionality and number of species has been studied. Such patterns are often found in systems where some quantity is conserved, so-called conservative systems, and because of this, conservation laws were sought in the investigated types of systems. Since the reactions taking place in biological systems are very situation specific, a more general mathematical approach was used. The foundation for the project was a method to find a conserved quantity along with a function representing the reaction mechanism for a one-dimensional one-species system.

It was found that the known method could not be straightforwardly generalized to higher spatial dimensionality. However, it was shown that when instead increasing the number of species for a one-dimensional system (where the function representing the reaction mechanism is some generalized version of that found in the known method), it is possible to find a conservation law similar to that for one species. Whether or not more than one conserved quantities could exist for the N-species case is unclear.

Once this conserved quantity was found, the connection between trajectories in phase space and quasi-periodic patterns along the spatial dimension of the system was studied. For the two-species case it was found that quasi-periodic patterns along the spatial dimension are possible. The stability of such patterns in time (under the actual RD-dynamics) is unclear, since the static "equations of motion" studied could result from dynamical equations other than those of RD.

It was shown, for the two-species case, that around each fixed point of the system there exist two local orthogonal planes spanning the local phase space. In each of these the dynamics is linearized. If the conserved quantity is seen as an energy, the distribution of energy between these two planes resembles that of two non-linearly coupled pendulums.

Possible extensions of the work done would be to (*i*) find out if there exist systems with more than one conserved quantity, (*ii*) study the time-stabilities of the found patterns under various dynamics and (*iii*) find applications in terms of real biological systems that can be described by the investigated kinds

of systems.

A Discretization of the continuous RD-equation

The continuous RD-equation for an n-dimensional system of one species in steady-state ($\partial_t u = 0$) is given by, for $u = u\left(\{x_i\}_{i\in\{1,2,\ldots,n\}}, t\right)$ and $\partial_i = \partial_{x_i}$,

$$0 = \nabla^2 u + F(u) = \sum_{i=1}^{n} \partial_i^2 u + F(u) \tag{87}$$

Now, for all $i, j \in \{1, 2, \ldots, n\}$, the discretization of $\partial_i^2 u$ looks exactly the same as that for $\partial_j^2 u$, the only difference being the respective step lengths. It therefore suffices to look at one such discretization in detail. The definition of the partial derivative of u with respect to component i is

$$\frac{\partial u}{\partial x_i} = \lim_{\Delta x_i \to 0} \frac{u\left(x_1, \ldots, x_i + \frac{1}{2}\Delta x_i, \ldots, x_n, t\right) - u\left(x_1, \ldots, x_i - \frac{1}{2}\Delta x_i, \ldots, x_n, t\right)}{\Delta x_i} \tag{88}$$

Using the definition again to obtain the second partial derivative gives

$$\begin{aligned} \frac{\partial^2 u}{\partial x_i^2} = \quad & \lim_{\Delta x_i \to 0} \left[\frac{u\left(x_1, \ldots, x_i + \Delta x_i, \ldots, x_n, t\right) - 2u\left(x_1, \ldots, x_i, \ldots, x_n, t\right)}{\left(\Delta x_i\right)^2} + \right. \\ & \left. + \frac{u\left(x_1, \ldots, x_i - \Delta x_i, \ldots, x_n, t\right)}{\left(\Delta x_i\right)^2} \right] \end{aligned} \tag{89}$$

The system can now be discretized according to

$$\begin{cases} x_i \longrightarrow x_i^{k_i} = k_i \Delta x_i, & \forall i \in \{1, \ldots, n\} \\ u \longrightarrow u^{k_1, \ldots, k_n} = u\left(\left\{x_j^{k_j}\right\}_{j\in\{1,\ldots,n\}}, t\right) \end{cases} \tag{90}$$

where the superscript of u shows that each k_i is independent of the others. Using this notation in the expression for the second partial derivative gives

$$\frac{\partial^2 u}{\partial x_i^2} \longrightarrow \frac{u^{k_1,\ldots,k_i+1,\ldots,k_n} + u^{k_1,\ldots,k_i-1,\ldots,k_n} - 2u^{k_1,\ldots,k_i,\ldots,k_n}}{\left(\Delta x_i\right)^2} \tag{91}$$

As can be seen, the structure of the numerator is the sum of nearest neighbors in the i-direction minus twice the value of u at the chosen point. Doing this for all directions, assuming that all of the step lengths are the same (i.e. $\Delta x_i = \Delta x_j \equiv a \ \forall i, j$), letting lattice point be denoted by l and defining $u_l \equiv u^{k_1,\ldots,k_n}$, yields the discretized RD-equation

$$0 \longrightarrow \frac{1}{a^2} \sum_{j\in\xi(l)} u_j - \frac{2n}{a^2} u_l + \tilde{F} \tag{92}$$

where $\tilde{F}$ is the discretized version of $F(u)$ and $\xi(l)$ is the set of nearest neighbors of u_l. Multiplying through by a^2 and absorbing all terms independent of nearest neighbors and $\tilde{F}$ into $f(u_l)$ gives

$$0 = \sum_{j\in\xi(l)} u_j - f(u_l) \tag{93}$$

which is the discretized RD-equation presented in the introduction.

B Matrix diagonalization

A well-known relation from linear algebra is that an $N \times N$-matrix $\mathbf{A}$ is diagonalizable if there exists some matrix $\mathbf{T}$ such that $\mathbf{T}^{-1}\mathbf{A}\mathbf{T} = \mathbf{\Lambda} = \mathrm{diag}(\mu_1, \mu_2, \ldots, \mu_N)$ for eigenvalues $\{\mu_j\}_{j\in\{1,2,\ldots,N\}}$ to matrix $\mathbf{A}$ with corresponding eigenvectors $\{\mathbf{v}_j\}_{j\in\{1,2,\ldots N\}}$. Rewriting the relation as $\mathbf{A}\mathbf{T} = \mathbf{T}\mathbf{\Lambda}$, it can be noted that if $\mathbf{T}$ is defined as having the eigenvectors $\{\mathbf{v}_j\}$ as columns, then the relation reduces to the simple expression $\mathbf{A}\mathbf{v}_j = \mu_j\mathbf{v}_j \ \forall j$.

If $\mathbf{T}$ is chosen to have the *normalized* eigenvectors of $\mathbf{A}$, $\{\hat{\mathbf{v}}_j\}$, as its columns, then $\mathbf{T}^\top\mathbf{T} = \mathbf{1}$, where $\mathbf{1}$ is the identity matrix of size $N \times N$. Also, since $\mathbf{T}^{-1} = \mathbf{T}^\top$, the matrix $\mathbf{T}$ is called orthogonal. A scalar product in the original space, $\mathbf{a}\cdot\mathbf{b}$ (for vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^N$), must transform as a scalar, i.e. $\mathbf{a}\cdot\mathbf{b} \to \mathbf{a}'\cdot\mathbf{b}' = \mathbf{a}\cdot\mathbf{b}$ where the primed vectors are in the new space. The relation between the new space and the old for a vector is $\mathbf{a}' = \mathbf{T}^{-1}\mathbf{a} = \mathbf{T}^\top\mathbf{a}$, and conversely for $\mathbf{b}'$. This gives $\mathbf{a}'\cdot\mathbf{b}' = \mathbf{a}^\top\mathbf{T}\mathbf{T}^\top\mathbf{b} = \mathbf{a}\cdot\mathbf{b}$, where the last equality follows from the choice of $\mathbf{T}$ as having the *normalized* eigenvectors as its columns[28].

C Perturbing the one-dimensional system

The onset of chaos in the one-dimensional one-species system is here studied. The function $f(u)$ for this system is

$$f(u) = \frac{Bu^2 - Du + E}{Au^2 - Bu + C} \tag{94}$$

for constants A, B, C, D and E. Note the special relation between the B's. The mapping in eq. (27) gives the fixed point relation, for fixed point (u, t),

$$2Au^3 - 3Bu^2 + (2C + D)u - E = 0 \tag{95}$$

Choosing $E = 0$ gives

$$0 = u\left(\frac{3B + \sqrt{9B^2 - 8A(2C + D)}}{4A}\right)\left(\frac{3B - \sqrt{9B^2 - 8A(2C + D)}}{4A}\right) \tag{96}$$

As can be seen, the origin is a fixed point no matter the values of the constants, whereas the positions of the other two clearly depend on them. Just as for the two-species system in sec. 3.2.5 the local Jacobian and hence the stabilities of the fixed points can be investigated. The eigenvalues λ to this Jacobian are

$$\lambda = \frac{1}{2}\left(\frac{df}{du} \pm \sqrt{\left(\frac{df}{du}\right)^2 - 4}\right) \tag{97}$$

[28] Of course, rows would work just as well.

and as should be noted, $\frac{df}{du} \in \{-2, 2\}$ for the fixed point to be elliptic. The derivative of $f(u)$ is easily calculated to be

$$\frac{df}{du} = \frac{1}{(Au^2 - Bu + C)^2} \left[u^2(DA - B^2) + 2uBC - DC\right] \tag{98}$$

For the origin this becomes

$$\left.\frac{df}{du}\right|_{u=0} = -\frac{D}{C} \tag{99}$$

For the origin to be a hyperbolic fixed point, D has to be chosen so that $D \geq 2C$ or $D \leq -2C$. For the set of parameter values

$$\begin{cases} A = 1 \\ B = 0.8 \\ C = 1 \\ D = -2.5 \\ E = 0 \end{cases} \tag{100}$$

the fixed points u become $u \in \{0, \approx 1.381, \approx -0.181\}$ such that $u = 0$ is hyperbolic and the other two elliptic. Now, introducing a perturbation ϵ in $f(u)$ such that

$$f(u) = \frac{Bu^2 - Du + E}{Au^2 - (B + \epsilon)u + C} \tag{101}$$

should destroy the integrability of the system for $\epsilon \neq 0$. When this perturbation is added, chaos should start appearing around the hyperbolic fixed point. Also, new cycle points should be created along the trajectories, and according to the Poincaré-Birkhoff theorem, there must be an equal number of created hyperbolic and elliptic cycle points for each such set of new cycle points. Around the new elliptic cycle points, regular trajectories should appear, thus forming "islands" in phase space. That new points are created in this way means that the structure in phase space could obtain a fractal structure (see e.g. [1]). All of this is studied in figs. 11– 15. All figures were created by randomly choosing a couple of hundred initial values on the diagonal between $(-1.5, -1.5)$ and $(1.5, 1.5)$ and then iterating the mapping in eq. (27) roughly one thousand times.

The figures show the following:

When the integrability of the system is destroyed, chaos sets in. It begins to appear around the hyperbolic fixed point, and for larger perturbations new cycle points and also islands of regular motion are created. The creation of such cycle points follows the Poincaré-Birkhoff theorem.

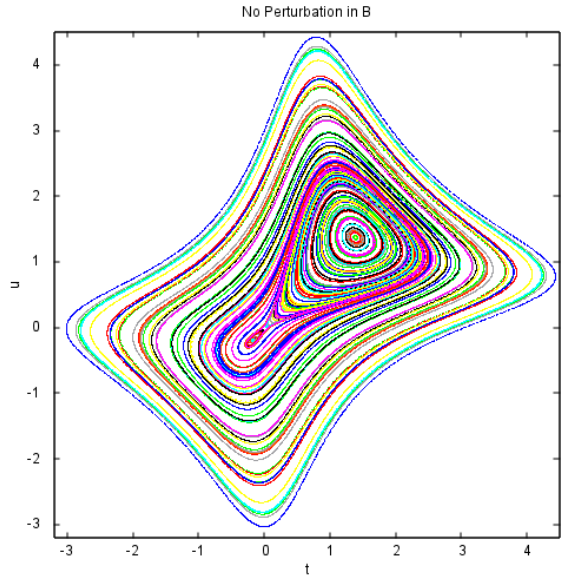

Figure 11: In this figure the created trajectories in phase space (u, t) are plotted. Here $\epsilon = 0$ and the three fixed points, the hyperbolic one (in the origin) and the elliptic two, can be seen. The trajectories are all periodic or quasi-periodic, as they should.

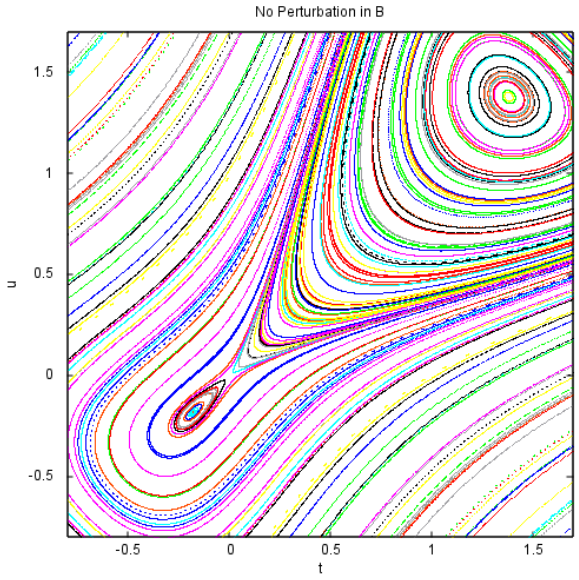

Figure 12: In this figure the created trajectories in phase space (u, t) are plotted. Here $\epsilon = 0$ again, but this figure shows a zoomed-in view of the structure in phase space. Here, the three fixed points can be seen.

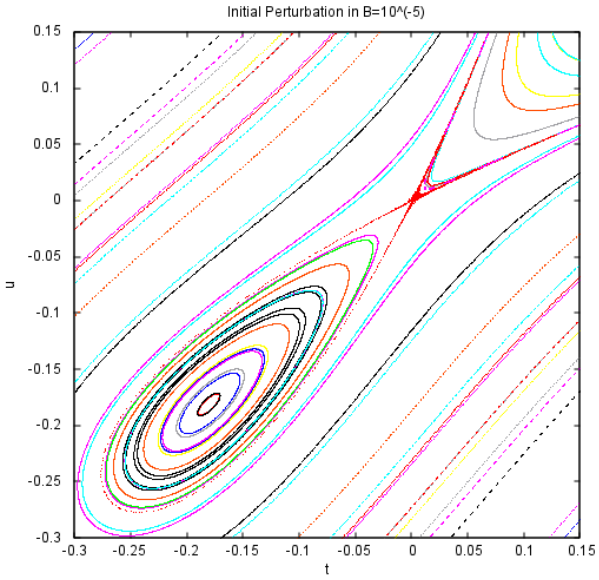

Figure 13: In this figure the created trajectories in phase space (u, t) are plotted. Here $\epsilon = 10^{-5}$. As can be seen, chaos has started to appear around the hyperbolic fixed point.

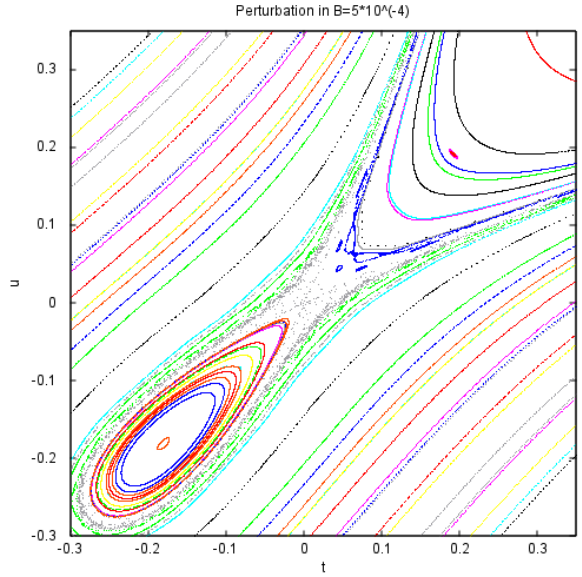

Figure 14: In this figure the created trajectories in phase space (u, t) are plotted. Here $\epsilon = 5 \cdot 10^{-4}$. As can be seen, chaos is obviously present in the system, as well as the emergence of new cycle points (the elliptical structures around the point $(0.08, 0.08)$). That such cycle points appear indicates the possibility of the structure being fractal.

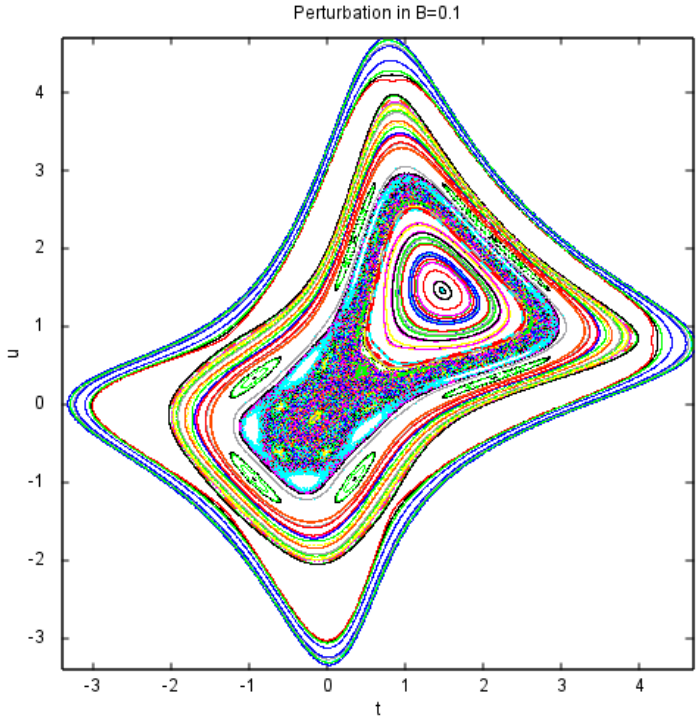

Figure 15: In this figure the created trajectories in phase space (u, t) are plotted. Here $\epsilon = 0.1$. Many "islands" of regular motion around new cycle points have been created. According to the Poincaré-Birkhoff theorem, the emergence of islands (elliptic cycle points) along a trajectory must be such that an equal number of hyperbolic and elliptic cycle points are created. Counting the number of, for one set of islands, created cycle points shows that this seems true.

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I would like to thank my parents, girlfriend and brother (with family) for all the support I have received and kindness I have been shown. Also my fellow thesis workers at the institution deserve some recognition, in particular for the interesting discussions on all things physics and mathematics. Last but not least I would like to thank my supervisor, Bo Söderberg, for the many inspiring and helpful meetings.

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