

# Limit cycles in the presence of convection, a first order analysis

E. H. FLACH<sup>1,2,3</sup>, S. SCHNELL<sup>3</sup> and J. NORBURY<sup>2</sup>

<sup>1</sup> Corresponding author: flach@indiana.edu

<sup>2</sup> Centre for Mathematical Biology,  
Mathematical Institute, 24-29 St Giles', Oxford, OX1 3LB, UK

<sup>3</sup> Indiana University School of Informatics, Complex Systems Group  
1900 East Tenth Street, Bloomington, IN 47406, USA

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## Abstract

We consider a diffusion model with limit cycle reaction functions. In an unbounded domain, diffusion spreads pattern outwards from the source. Convection adds instability to the reaction-diffusion system. We see the result of the instability in a readiness to create pattern. In the case of strong convection, we consider that the first-order approximation may be valid for some aspects of the solution behaviour. We employ the method of Riemann invariants and rescaling to transform the reduced system into one invariant under parameter change. We carry out numerical experiments to test our analysis. We find that most aspects of the solution do not comply with this, but we find one significant characteristic which is approximately first order. We consider the correspondence of the Partial Differential Equation with the Ordinary Differential Equation along rays from the initiation point in the transformed system. This yields an understanding of the behaviour.

*Keywords: reaction, diffusion, convection, limit cycle, Schnakenberg*

## 1 Introduction

Reaction-diffusion systems are of interest because of the many applications in biology. It is the formation of pattern that is the major motivation for study. For this reason, reaction mechanisms which can produce limit cycles are particularly significant. Schnakenberg [1] found the chemical pathway which yields the algebraically simplest set of functions which can produce a limit cycle. We employ these functions in a system with diffusion, representing Brownian motion. We add convection, which destabilises the system: pattern is formed more readily.

We carry out an extended first-order analysis, simplifying and rescaling the system to reduce it to its essential form. From this we see clearly how to identify first-order attributes of the generated pattern. We carry out numerical experiments to discover these aspects. We find that most attributes have a strong second-order component. Then we interpret the first-order result with the help of some more theory.

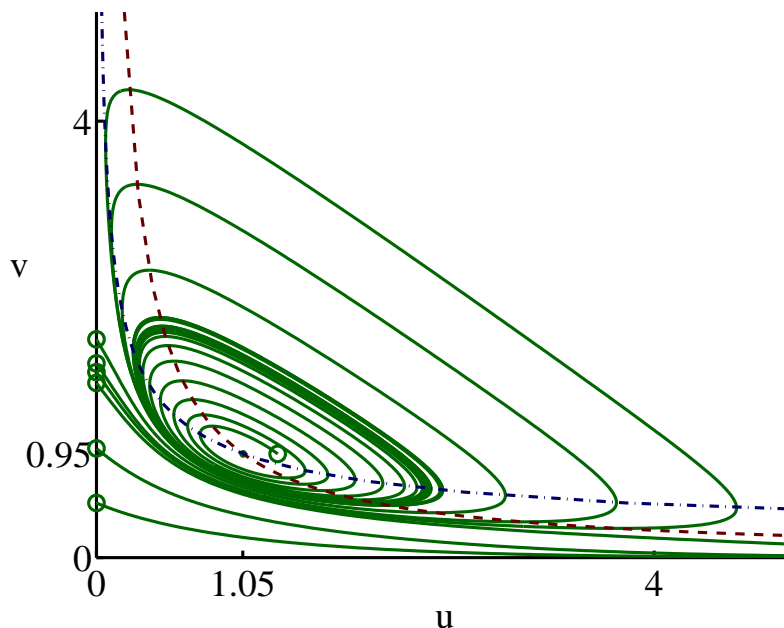


Figure 1: Phase space for the limit-cycle reaction, given by numerical solution of (2). The phase curves spiral out from the steady state to meet the limit cycle (the broad loop). The trajectories starting high on the  $v$ -axis spiral into the limit cycle. There is a separatrix below which the limit cycle is no longer the attractor and all trajectories head off to  $(u, v) = (\infty, 0)$ . Solid curves starting with circles are the trajectories. The dashed line is the  $uv = 1$  nullcline, the dash-dotted is  $uv^2 = \mu$ . The parameter here is  $\mu = 0.95$ .

## 2 Limit cycles

We suppose that some form of chemical reaction is the underlying basis for biological pattern formation. The Schnakenberg reaction is a simple chemical system that is known to have cyclic behaviour. This is a self-catalysing chemical reaction, also known as an autocatalytic reaction. Limit cycle solutions can exist in this type of two-species system (see Hanusse [2] and Tyson and Light [3]). The reaction functions are

$$\begin{aligned} f &= \mu - uv^2, \\ g &= uv^2 - v, \end{aligned} \tag{1}$$

with  $\mu$  the constant, positive source term.

If the reaction is homogeneous, an ODE is an appropriate model:

$$\begin{aligned} u' &= f, \\ v' &= g. \end{aligned} \tag{2}$$

We note that this is a one-parameter model:  $\mu$  determines the behaviour of the system.

We examine the behaviour of the model. There is one finite steady state:  $(1/\mu, \mu)$ . With a linear stability analysis we see that the steady state is stable for  $\mu > 1$ , and unstable for  $\mu < 1$ . Furthermore, in the range  $3 - 2\sqrt{2} < \mu^2 < 3 + 2\sqrt{2}$  ( $0.4 \lesssim \mu \lesssim 2.4$ ), there will be oscillatory behaviour.

The linear theory cannot tell all aspects of the system. Merkin et al. [4] found limit cycle behaviour in the range  $0.90032 \approx \mu_* < \mu < 1$ . We are interested in this behaviour

(see FIGURE 1). The steady state is where the two nullclines (the broken lines in the diagram) cross. The circled points on the diagram show the start of the phase plane trajectories. The phase curves spiral out from the steady state to meet the limit cycle (the broad loop in the diagram). The trajectories starting high on the  $v$ -axis spiral into the limit cycle. There is a separatrix below which the limit cycle is no longer the attractor and all trajectories head off to  $(u, v) = (\infty, 0)$ , a globally stable steady state. The special value  $\mu_*$  occurs when the limit cycle grows so much that it meets the separatrix, and then the limit cycle breaks.

### 3 Diffusion and convection

Biological pattern formation is by definition spatially differentiated [5]. There are many models for this. We choose the simplest case: one spatial dimension and some diffusion. The diffusion corresponds to the averaged gross effect of random motion, and with passive movement is equivalent to Brownian motion.

We add a convective term to the system. A change of coordinates can be employed to remove the convection on one of the species. In the case where the convection is the same strength on both, it is completely removable. So we consider different convection on each species:

$$\begin{aligned} u_t &= \varepsilon_1 u_{xx} + f , \\ v_t &= \varepsilon_2 v_{xx} - \gamma v_x + g , \end{aligned} \tag{3}$$

with  $f$  and  $g$  as in (1) and  $\varepsilon_1$ ,  $\varepsilon_2$  and  $\gamma$  positive constants.

### 4 Pattern formation

We have reaction functions that have limit-cycle behaviour and convection which is known to drive instability. The appearance of pattern is then to be expected, although the form might be more difficult to predict. Satnoianu et al. [6] studied this system (3) previously and found that periodic behaviour is emergent in the system over a broad parameter range.

In the numerical experiment, we start at the steady state  $(1/\mu, \mu)$ , except for a small disturbance at  $x = 0$ . We try to simulate a boundless environment – to this end we find zero derivative boundary conditions the most effective. The initial disturbance propagates and becomes pronounced, forming a regular pattern with aligned oscillations. The propagation is linear, forming a V-shape. We see a difference in behaviour between the left and right sides of the pattern (FIGURE 2): the angle of alignment and the frequency of the pattern is different on either side. This pattern is the main focus of our study.

### 5 First-order analysis

We approximate the full system (3) with the first order differential system:

$$\begin{aligned} u_t &= f , \\ v_t &= -\gamma v_x + g . \end{aligned} \tag{4}$$

We look for the characteristic directions, also known as Riemann invariants, of this first order system. We make a change of variables into this new canonical coordinate system:

$$\xi = t - \frac{x}{\gamma}, \quad \eta = \frac{x}{\gamma} . \tag{5}$$

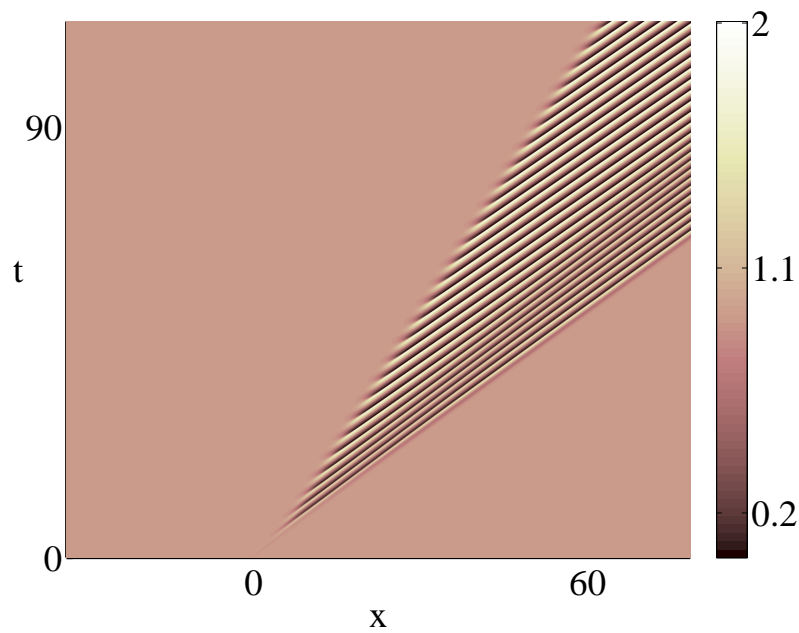


Figure 2: Pattern found for a diffusion system with convection and limit-cycle reaction kinetics (3). The initial disturbance propagates and becomes pronounced, forming a regular pattern with aligned oscillations. The propagation is linear, forming a V-shape. There is a difference in behaviour between the left and right sides of the pattern: the angle of alignment and the frequency of the pattern is different on either side. This is a numerical solution using NAG D03PCF, plotting species  $u$  with  $\gamma = 1$ ,  $\varepsilon_1 = 0.01$ ,  $\varepsilon_2 = 0.01$ ,  $\mu = 1.1$ . The reactants are initially at steady state:  $(u, v) = (1/\mu, \mu)$ , with a small disturbance at  $x = 0$ . The boundaries are held at zero derivative:  $u_x, v_x = 0$ .

This transformation has one limitation:  $\gamma$  may not be equal to zero. The new coordinates becomes undefined for this value, so there is a possible discontinuity in the system behaviour as convection is introduced. This distances our analysis from the standard reaction-diffusion systems used in pattern formation.

The ordering  $(x, t) \rightarrow (\xi, \eta)$  implies a reflection in the plane, and so left and right are transposed in the canonical system. The transformed first order differential system (4) is as follows:

$$\begin{aligned} u_\xi &= f, \\ v_\eta &= g. \end{aligned} \tag{6}$$

We have succeeded in reducing the system by one differential term and separated the independent variables, each now having their own equation. Further, we have removed the parameter  $\gamma$  through the implicit rescaling. Note that the method of characteristics unfortunately has not separated the dependent variables in the reaction functions in this case.

Rescaling is one of the simplest and strongest tools available: the technique can reveal insights into system behaviour [7]. We introduce rescaled variables as follows:

$$u = \frac{\bar{u}}{k}, \quad v = k\bar{v}, \quad \mu = k\bar{\mu}. \tag{7}$$

This results in transformed reaction functions:

$$\begin{aligned} f &= k\bar{f}, \\ g &= k\bar{g}, \end{aligned} \tag{8}$$

with the transformed functions defined in the natural way. Now we consider the differential form (6). We choose suitable rescalings for the independent variables:

$$\xi = \frac{\bar{\xi}}{k^2}, \quad \eta = \bar{\eta}. \tag{9}$$

The transformed canonical equations are:

$$\begin{aligned} \bar{u}_{\bar{\xi}} &= \bar{f}, \\ \bar{v}_{\bar{\eta}} &= \bar{g}. \end{aligned} \tag{10}$$

If we choose  $k = \mu$  the system is now invariant under the parameter  $\mu$  ( $\bar{\mu} = 1$ ).

We take the pattern found previously (FIGURE 2) and apply the above coordinate change and rescaling. This results in a clearer view of the system behaviour (FIGURE 3).

## 6 Numerical experiments

We wish to see to what extent the behaviour of the full system (3) is an effect of only the first-order system (4). To this end, we choose strong convection, relative to the diffusion:  $\gamma \gg \varepsilon_1, \varepsilon_2$ . We choose the rescaling parameter  $k = \mu$ , which rescales  $\mu$  to 1. We carry out the simulation in the original system, with a range of values of  $\mu$ .

We take the results, transform them into a canonical coordinate system and then rescale them, producing a system theoretically invariant to  $\mu$ , to first order (10). We examine aspects of the system: the edges of the pattern, the alignment of the waves, their

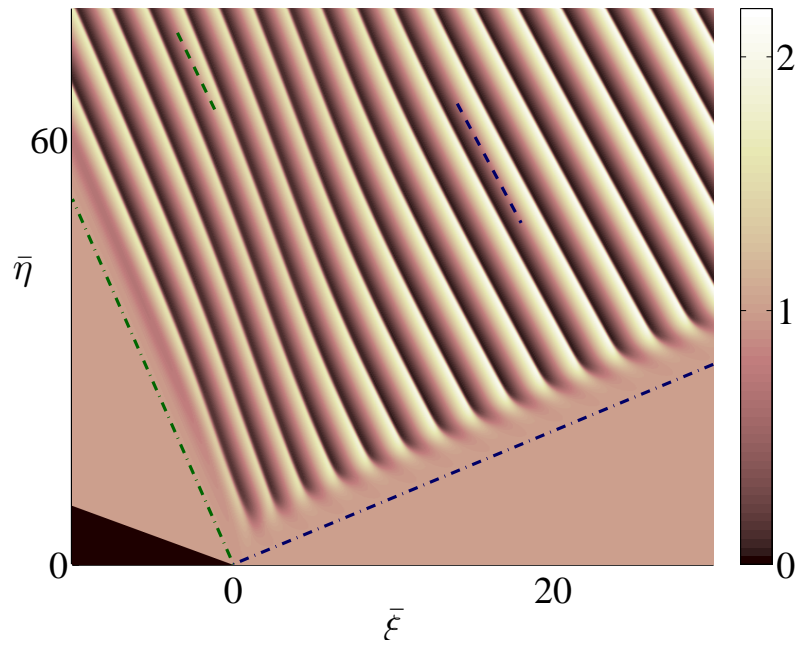


Figure 3: Canonical form of pattern. This is a diffusion system with convection and limit-cycle reaction kinetics (3), shown in transformed variables. There is little qualitative difference from the original coordinate system, but the pattern is clearer. The dash-dotted lines mark the edge of the pattern. The dashed lines mark the angle of the oscillation. This is a numerical solution using NAG D03PCF, plotting species  $\bar{u}$  with  $\gamma = 1$ ,  $\varepsilon_1 = 0.01$ ,  $\varepsilon_2 = 0.01$ ,  $\mu = 1.1$ . The reactants are initially at steady state:  $(u, v) = (1/\mu, \mu)$ , with a small disturbance at  $x = 0$ . The boundaries are held at zero derivative:  $u_x, v_x = 0$ .

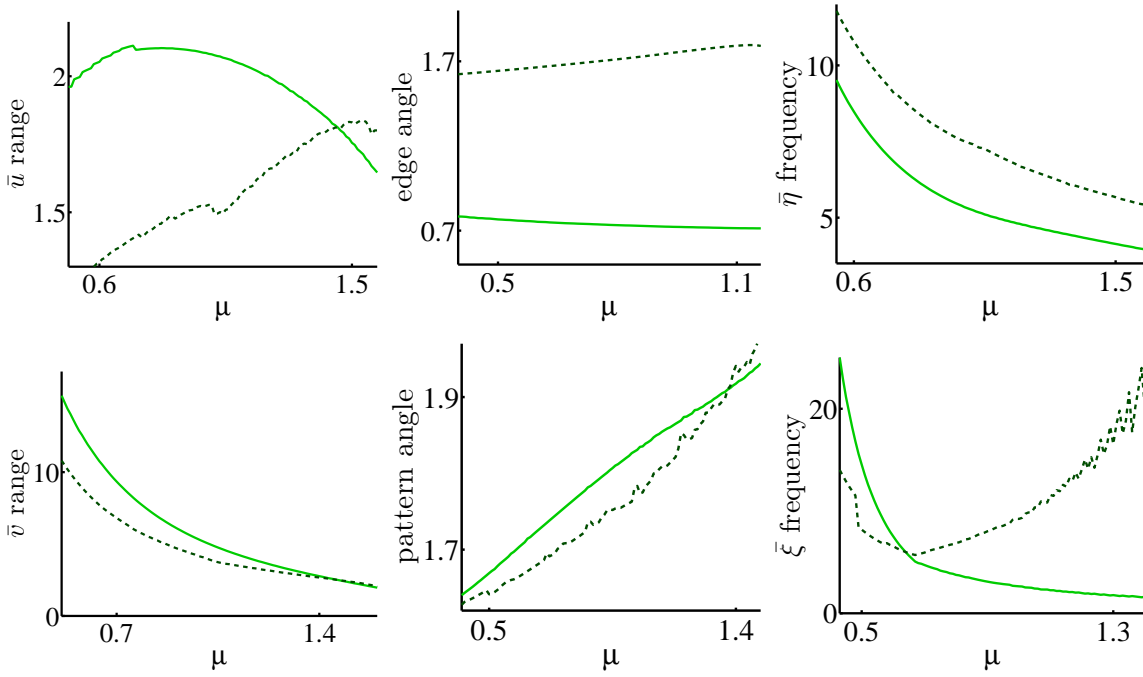


Figure 4: Pattern behaviour as a function of the reaction parameter: measurable aspects of the pattern collated over a large range of  $\mu$ . The lighter, solid lines are measurements from the left side of the pattern (right in the canonical coordinates), the darker, broken lines from the right. Pattern is found for the diffusion system with convection and limit-cycle reaction kinetics (3). Numerical simulations were run at 0.1 intervals of  $\mu$ , using NAG D03PCF, with  $\gamma = 1$ ,  $\varepsilon_1 = 0.01$  and  $\varepsilon_2 = 0.01$ . Measurements were taken in the transformed system. The reactants are initially at steady state:  $(u, v) = (1/\mu, \mu)$ , with a small disturbance at  $x = 0$ . The boundaries are held at zero derivative:  $u_x, v_x = 0$ .

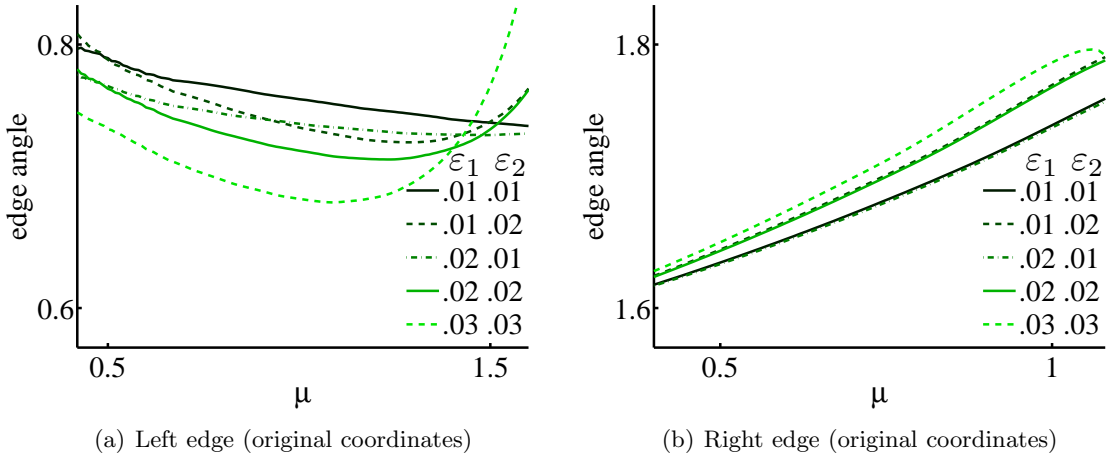


Figure 5: Edge behaviour over a range of diffusion. The right edge is clearly increasing, perhaps linearly. The left edge has a limited range, reducing with  $\epsilon_1$  and  $\epsilon_2$ . Pattern is found for the diffusion system with convection and limit-cycle reaction kinetics (3). Numerical simulations were run at 0.1 intervals of  $\mu$ , using NAG D03PCF, with  $\gamma = 1$ . Measurements were taken in the transformed system. The reactants are initially at steady state:  $(u, v) = (1/\mu, \mu)$ , with a small disturbance at  $x = 0$ . The boundaries are held at zero derivative:  $u_x, v_x = 0$ . The dotted line is  $\pi/4$ .

amplitude and frequency. The transformed pattern and some of these measurements are shown in FIGURE 3.

We collate the measurements (FIGURE 4) and analyse the behaviour of the pattern. If any aspect of the pattern is a first order effect, then we expect it to remain constant under the transformation. Our results show various responses to variation of  $\mu$ . Of all the measurements we make, only the edge angles of the pattern could possibly be close to constant.

We examine the behaviour of the edge angle in more detail, exploring other values for the diffusion constants  $\epsilon_1$  and  $\epsilon_2$  (FIGURE 5). We see that the right edge angle is roughly increasing with  $\mu$ , perhaps linearly, and so cannot be a constant attribute. The left edge angle is more difficult to characterise. However, for smaller amounts of diffusion the range of values becomes quite small. We claim that this curve is approximately constant. Since we know the system is actually second-order, we can consider this specific behaviour to be approximately first-order.

## 7 Correspondence of the PDE with the ODE

We consider a curve in  $\xi, \eta$  space parameterised by  $s$ . We consider rays emanating from the origin:  $\eta = s = a\xi$ . This gives us the derivative along the curve:

$$\begin{aligned} \frac{du}{ds} &= \frac{1}{a} \frac{\partial u}{\partial \xi} + \frac{\partial u}{\partial \eta}, \\ \frac{dv}{ds} &= \frac{1}{a} \frac{\partial v}{\partial \xi} + \frac{\partial v}{\partial \eta}. \end{aligned} \tag{11}$$

Since  $(u, v)$  is a solution of the transformed first order equation (6), we can substitute some of the partial derivatives.

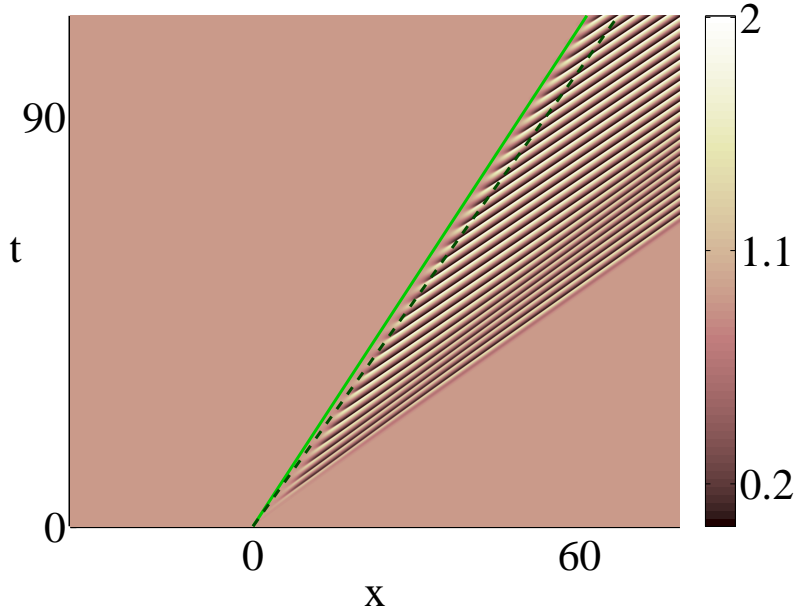


Figure 6: ODE correspondence. The lines indicate the range of existence of the limit cycle in the ODE, mapped onto the PDE by considering rays from the origin in the canonical system. The lighter, solid line is at the Hopf bifurcation point in the ODE, and very close to the onset of the PDE pattern. The pattern is found for a diffusion system with convection and limit-cycle reaction kinetics (3). This is a numerical solution using NAG D03PCF, plotting species  $u$  with  $\gamma = 1$ ,  $\varepsilon_1 = 0.01$ ,  $\varepsilon_2 = 0.01$  and  $\mu = 1.1$ . The reactants are initially at steady state:  $(u, v) = (1/\mu, \mu)$ , with a small disturbance at  $x = 0$ . The boundaries are held at zero derivative:  $u_x, v_x = 0$ .

We make a strong assumption:  $u_\eta = 0 = v_\xi$ . This is a substantial restriction to the system. However zero is the natural, or first, value to consider for these terms. The need for this assumption to fully determine the system arises because we are trying to examine the system without the effect of the boundaries.

This reduces the first-order PDE to the ODE system:

$$\begin{aligned} a \frac{du}{ds} &= f, \\ \frac{dv}{ds} &= g. \end{aligned} \tag{12}$$

We rescale the variables similarly to before, to remove the constant  $a$ . We set  $u = \hat{u}/\sqrt{a}$ ,  $v = \sqrt{a}\hat{v}$ ,  $\mu = \sqrt{a}\hat{\mu}$ ,  $s = \hat{s}$ . This recovers the natural ODE:

$$\begin{aligned} \frac{d\hat{u}}{d\hat{s}} &= \hat{f}, \\ \frac{d\hat{v}}{d\hat{s}} &= \hat{g}. \end{aligned} \tag{13}$$

This gives the correspondence between  $\hat{\mu}$  in the rescaled ODE and  $\mu$  in the PDE together with the ray angle  $a$  ( $\mu = \sqrt{a}\hat{\mu}$ ). The range of existence of the limit cycle in the ODE ( $\mu_\star < \hat{\mu} < 1$ ) is then used to predict the range of existence of the stable oscillations

in the PDE:

$$\mu^2 < a < a_\star \equiv \frac{\mu^2}{\mu_\star^2}, \quad (14)$$

for the ray angle  $a$  in the canonical coordinate system. In the original coordinate system  $(x, t)$  we have:

$$1 + \frac{\mu_\star^2}{\mu^2} \equiv h_\star < h < 1 + \frac{1}{\mu^2}, \quad (15)$$

where  $h$  is the gradient of the ray,  $t = hx$ . For our example value ( $\mu = 1.1$ ) we have  $1.67 \lesssim h \lesssim 1.82$ .

For  $\hat{\mu} = 1$  we have the onset of the instability in the ODE, and we can expect this behaviour to remain fixed in the PDE. We do indeed see a close match between the predicted value for the onset of the pattern,  $h = 1 + 1/\mu^2$ , and the actual gradient of the initiation of the pattern (FIGURE 6).

The other bound is almost within the transition behaviour of the onset, and certainly a long way from the other edge. As  $\hat{\mu}$  increases beyond  $\mu_\star$  we still have oscillatory behaviour in the system, which suggests that the lower ODE bound is more flexible in the PDE system. We have previously observed [8] that the existence of this controlled type of behaviour is likely to be a result of the bounds introduced by Schnakenberg to constrain the trajectories into a limit cycle. It seems that these bounds apply more generally in the extended system.

In the original coordinate system we see that this prediction corresponds to the left edge of the pattern (in canonical coordinates this is the right edge). This was the aspect of the pattern that gave the strongest indication of being a first order effect in our experiments. In our rescaled canonical system,  $\bar{\mu} = 1$  and so  $a = 1$ , which is  $\pi/4$  radians as an angle. If we return to the experiment (FIGURE 5), we see that this value, roughly 0.785, is a good approximation to our results.

## 8 Discussion

We have been fortunate to find the initiation of the pattern as a first-order effect. Of all the attributes of the ODE, this is the most clear and significant. Finding an exact formula for this angle justifies the extensive analysis, and the close correspondence to the pattern formed by the PDE is pleasing.

As for the other edge: the theoretical prediction was weak and the behaviour here is not first-order from computer experiments. We should also note that the behaviour to the left of the left edge also corresponds to the first order analysis, in that it remains stable. In contrast, we would expect rays from the origin to the right of the right edge to be highly unstable, in the first order analysis.

The main significance of the result is that without this work we could not distinguish clearly between the two edges of the pattern. A second-order linear stability analysis would not readily differentiate between the two. The use of numerical simulations to establish the analytical result is absolutely vital.

The other measurements concern the established pattern. We have seen that almost every measurable aspect of the pattern does not correspond to first-order behaviour. The behaviour within the pattern is far from the steady state and so clearly non-linear.

Much of the theoretical analysis here relies on the rescalability of the reaction functions. This quality does not generally hold for less algebraically neat functions, however an approximation could be considered in this case.

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