The Gray-Scott (GS) model describes a chemical reaction-diffusion system which supports a wide variety of patterns, including localized pulses (1-D) and spots (2-D) which have been observed numerically and in experiment. As we will describe below, the system also supports the dynamic process of "pulse-splitting", which may be thought of as the reverse of the coarsening process seen in many pattern forming systems. For the regime we will consider, the governing equations are

$$\begin{aligned} \frac{\partial U}{\partial t} &= \nabla^2 U - UV^2 + A(1-U) \\ \frac{\partial V}{\partial t} &= \delta^2 \nabla^2 V + UV^2 - BV \end{aligned}$$

U and V are scalar fields representing chemical concentrations. A and B are parameters describing the feed of u and v from an external reservoir with fixed concentrations $u = 1$ and $v = 0$. $\delta^2 << 1$ represents the ratio of their diffusion coefficients.

We make the travelling wave ansatz $u, v = u(\zeta), v(\zeta)$, $\zeta = x - ct$. This yields

$$
\begin{aligned}
u' &= p \\
p' &= -cp + uv^2 - A(1-u) \\
\delta v' &= q \\
\delta q' &= -\frac{c}{\delta} q - uv^2 + Bv
\end{aligned}
$$

Set $\zeta = \delta\eta$, $c = \delta\gamma$ to obtain

$$
\begin{aligned}
\dot{u} &= \delta p \\
\dot{p} &= \delta \left[-\delta\gamma p + uv^2 - A(1-u) \right] \\
\dot{v} &= q \\
\dot{q} &= -\gamma q - uv^2 + Bv
\end{aligned}
$$

Observe the natural separation of the system into **fast** (v, q) and **slow** (u, p) subsystems.

We apply 3 criteria for rescaling:

- Scale making use of numerically determined pattern rich parameter regimes
- Maintain the fast/slow separation of scales in the system.
- Look for homoclinic orbits and saddle points with small friction γ

This suggests

$$\boxed{\begin{array}{ccc} A = \delta^2 a & B = \delta^{\frac{2\alpha}{3}} b & c = \delta^{1+\beta}\widehat{\gamma} \\ u = \delta^{\alpha}\widehat{u} \quad p = \delta^{\frac{2\alpha}{3}}\widehat{p} & v = \delta^{-\frac{\alpha}{3}}\widehat{v} & q = \widehat{q} \end{array}}$$

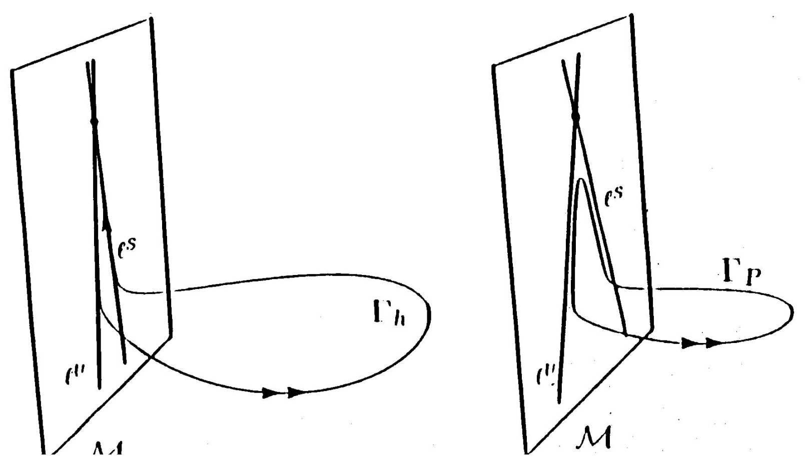
where $0 \leq \alpha < \frac{3}{2}$ and $\frac{1}{2} < 2-\alpha \leq \beta$. The results discussed apply only in this regime, but an upcoming papers discusses how these solutions may be extended to other regions in the parameter space[1]. In what follows we assume all the rescaled quantities are $O(1)$.

[1] A. Doelman, W. Eckhaus, and T.J. Kaper (1998), submitted

For convenience define $\epsilon = \delta^{1-\frac{2\alpha}{3}}$, $\epsilon^{2+\sigma} = \delta^{\beta-\frac{\alpha}{3}}$, $\delta = \epsilon^{\rho}$. Substituting and dropping hats

$$\boxed{\begin{aligned}
\dot{u} &= \epsilon p \\
\dot{p} &= \epsilon\left[uv^2 - \epsilon^{\frac{1}{2}(3\rho+1)}a - \epsilon^{(2\rho+1+\sigma)}\gamma p + \epsilon^{(3\rho-1)}au\right] \\
\dot{v} &= q \\
\dot{q} &= -uv^2 + bv - \epsilon^{(2+\sigma)}\gamma q
\end{aligned}}$$

In this way a system with 3 free parameters (A, B, c) becomes a system with 5 free parameters $(a, b, \gamma, \sigma, \rho)$. We use the extra freedom to show geometrically that periodic/homoclinic solutions to this system exist.



Consider the **fast subsystem**

$$
\begin{aligned}
\dot{v} &= q \\
\dot{q} &= -uv^2 + bv - \epsilon^{(2+\rho)}\gamma q
\end{aligned}
$$

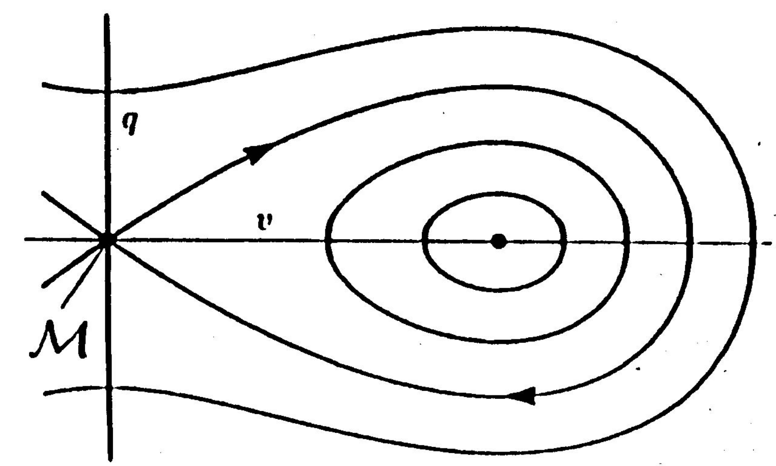
For $\epsilon = 0$ there is the Hamiltonian

$$\boxed{K = \frac{q^2}{2} - \frac{b}{2}v^2 + \frac{1}{3}uv^3}$$

We have a saddle point at $(0,0)$ connected by the homoclinic orbit

$$v_0 = 3b/(2u_0)sech^2(\sqrt{b}t/2), \qquad q_0 = \dot{v_0}$$

Observe that $u = u_0 = constant$ to leading order in the fast subsystem.



Consider the **slow subsystem**

$$\begin{aligned} u' &= p \\ p' &= -\epsilon^{\frac{1}{2}(3\rho+1)}a - \epsilon^{(2\rho+1+\sigma)}\gamma p + \epsilon^{(3\rho-1)}au \end{aligned}$$

For $\epsilon > 0$ there is the saddle point $(u_s, p_s) = (\epsilon^{-\frac{3}{2}(\rho-1)}, 0)$. Linearizing yields the eigenvalues $(\lambda_\pm)$ and eigenvectors

$$\begin{aligned} \lambda_\pm &= \frac{1}{2}\epsilon^{\frac{1}{2}(3\rho-1)}\left[\pm\sqrt{4a + \epsilon^{(\rho+3+2\sigma)}\gamma^2} - \epsilon^{(\rho+3+2\sigma)}\gamma\right] \\ p &= \lambda_\pm (u - u_s) \end{aligned}$$

For $\rho > 1$, $u_s >> 1$ yielding the approximate the stable and unstable directions

$$\boxed{\ell^{U,S} : \qquad p = \pm\epsilon\sqrt{a} + h.o.t.}$$

To understand the transition from $\epsilon = 0$ dynamics to $\epsilon \neq 0$ dynamics in the system, consider the generic problem

$$\begin{aligned} x' &= f(x, y, \epsilon) \\ y' &= \epsilon g(x, y, \epsilon) \end{aligned}$$

where $x, y \in \Re^{n,m}$, respectively. Now let $\epsilon \to 0^+$ to obtain

$$\begin{aligned} x' = f(x, y, 0) \\ y' = 0 \end{aligned}$$

This is exactly the fast subsystem case. We obtain a reduced dynamics on the fast manifold $y = constant$. Observe that even if $0 < \epsilon << 1$, the "leading order behavior" of the fast subsystem remains unaffected, even though the dynamics of y are no longer trivial. This regime is analagous to the "inner" (fast) solution of a singular perturbation/boundary layer problem.

Alternatively, introduce $\tau = \epsilon t$ to obtain

$$\begin{aligned} \epsilon x' &= f(x, y, \epsilon) \\ y' &= g(x, y, \epsilon) \end{aligned}$$

Now let $\epsilon \to 0^+$ to obtain

$$\begin{aligned} f(x, y, 0) &= 0 \\ y' &= g(x, y, 0) \end{aligned}$$

This is exactly the slow subsystem case. We obtain the slow dynamics confined to the **slow manifold** $M_0 \equiv f(x, y, 0) = 0$. This regime is analogous to the "outer" (slow) solution of a singular perturbation/boundary layer problem. To understand what happens to the slow manifold for $0 < \epsilon << 1$ we invoke the Fenichel theorems of geometric singular perturbation theory.

We summarize Fenichel's theorems: For sufficiently small ϵ

- there exists a manifold M_ϵ within $\mathrm{O}(\epsilon)$ of M_0 which is diffeomorphic to M_0 and locally invariant under the slow flow.

- there exist manifolds $W^s(M_\epsilon)$ and $W^u(M_\epsilon)$, locally invariant under the slow flow, that lie within $\mathrm{O}(\epsilon)$ of, and are diffeomorphic to, $W^s(M_0)$ and $W^u(M_0)$, respectively.

- trajectories on $W^s(M_\epsilon)$ $(W^u(M_\epsilon))$, approach (depart) M_ϵ at an exponential rate.

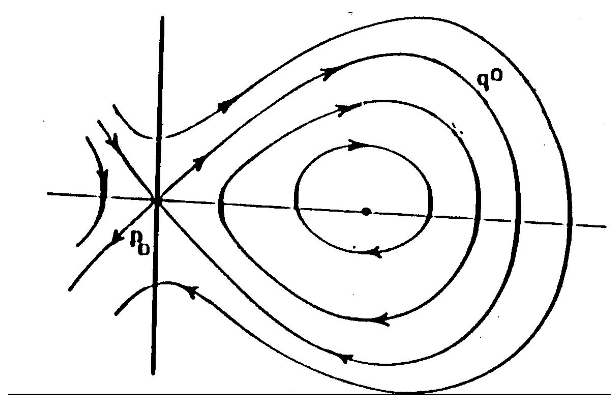
In the present case the slow manifold is given by $M_0 \equiv (u, p, v = q = 0)$, where every point of the (u, p) plane is the saddle point base of a fast homoclinic orbit. By the Fenichel theorems for $0 < \epsilon << 1$ there persists a perturbed slow manifold M_ϵ which is connected to the fast subsystem via exponentially decaying/growing orbits. Note that the dynamics on M_ϵ is no longer trivial, but that the Fenichel theorems allow us to maintain the separation of fast and slow subsystems.

Now to understand what happens to the fast subsystem we need to apply Melnikov's method. Melnikov's method is used to measure the "splitting distance" between the perturbed stable and unstable manifolds of a homoclinic orbit in a planar Hamiltonian system. As a generic example, consider the system

$$\dot{x} = f_1(x, y) = \frac{\partial H}{\partial y} + \epsilon g_1(x, y, t)$$

$$\dot{y} = f_2(x, y) = -\frac{\partial H}{\partial x} + \epsilon g_2(x, y, t)$$

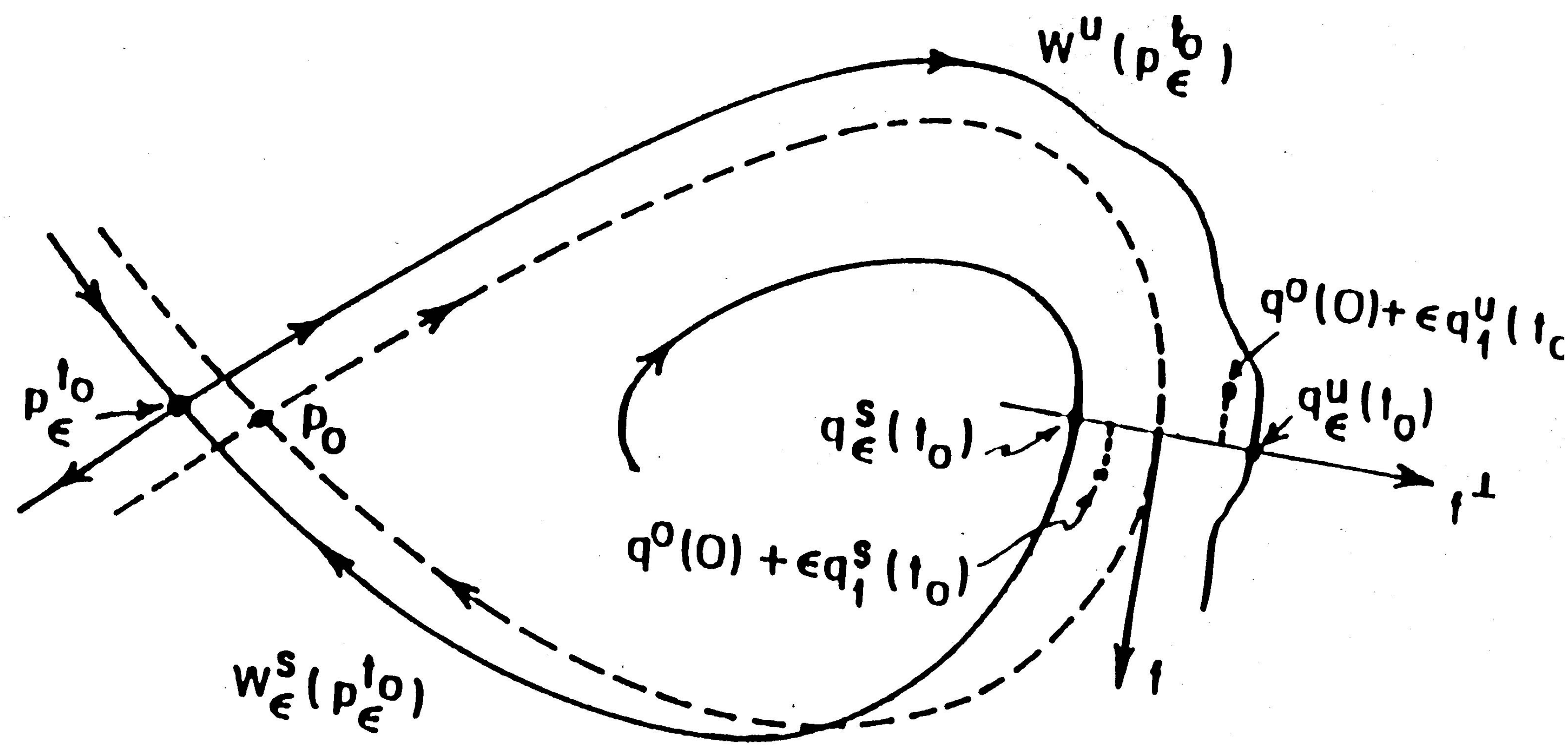
where H is the Hamiltonian. Assume the system possesses a homoclinic orbit $(x(s), y(s))$ for $\epsilon = 0$. We do not expect the homoclinic orbit to survive the perturbation. So to measure the distance between the stable and unstable manifolds, project the flow as follows.



When $\epsilon = 0$, the flow follows the path $F = (\partial_y H, \, -\partial_x H)^T$ at every point in phase space. For a small perturbation we linearize about that homoclinic orbit and project onto the normal to F, $F^\perp = (\partial_x H, \, \partial_y H)$. Integrate over time to determine the Melnikov function ΔK

$$\begin{aligned}
\epsilon \Delta K &= \int_{-\infty}^{\infty} dt \left(\frac{\partial H}{\partial x}, \, \frac{\partial H}{\partial y} \right) \cdot \left(\begin{array}{c} f_1(x,y) \\ f_2(x,y) \end{array} \right) \Bigg|_{(x(s),y(s))} \\
&= \epsilon \int_{-\infty}^{\infty} dt \left(\frac{\partial H}{\partial x}, \, \frac{\partial H}{\partial y} \right) \cdot \left(\begin{array}{c} g_1(x,y,t) \\ g_2(x,y,t) \end{array} \right) \Bigg|_{(x(s),y(s))} \\
&= \epsilon \int_{-\infty}^{\infty} dt \dot{H} \Bigg|_{(x(s),y(s))} \\
\Rightarrow & \quad \boxed{\Delta K = \int_{-\infty}^{\infty} dt \dot{H} \Bigg|_{(x(s),y(s))}}
\end{aligned}$$

If the Hamiltonian represents "energy," then the Melnikov function represents the difference in energy between trajectories on the stable and unstable manifolds. For our purposes the important feature to note is that at points where the Melnikov function is 0, transversal intersections of the stable and unstable manifolds occur – i.e., a homoclinic orbit is formed.



In the GS model the Melnikov function is given by

$$\begin{aligned}
\Delta K &= \int_{-\infty}^{\infty} \dot{K}\,dt \\
&= \int_{-\infty}^{\infty} \left[-\epsilon^{(2+\sigma)}\gamma q^2 + \frac{1}{3}\epsilon p v^3\right] dt \\
&= \epsilon^2 \left(\frac{6b\sqrt{b}}{5u_0^2}\right)\left(\frac{2\widehat{p_0}}{u_0} - \epsilon^\sigma \gamma\right) + h.o.t.
\end{aligned}$$

where we have approximated $u = u_0, p = \epsilon\widehat{p_0}, v = v_0, q = q_0 + h.o.t.$ so that we enter the fast subsystem near the unstable eigendirection ℓ^U of the slow subsystem. Intersections may therefore occur along

$$\boxed{p = \tfrac{1}{2}\epsilon^{(1+\sigma)}\gamma u}$$

Finally, we may calculate the "change during flight", the influence of the fast subsystem on the value of p during the fast excursion. Straightforward computation yields

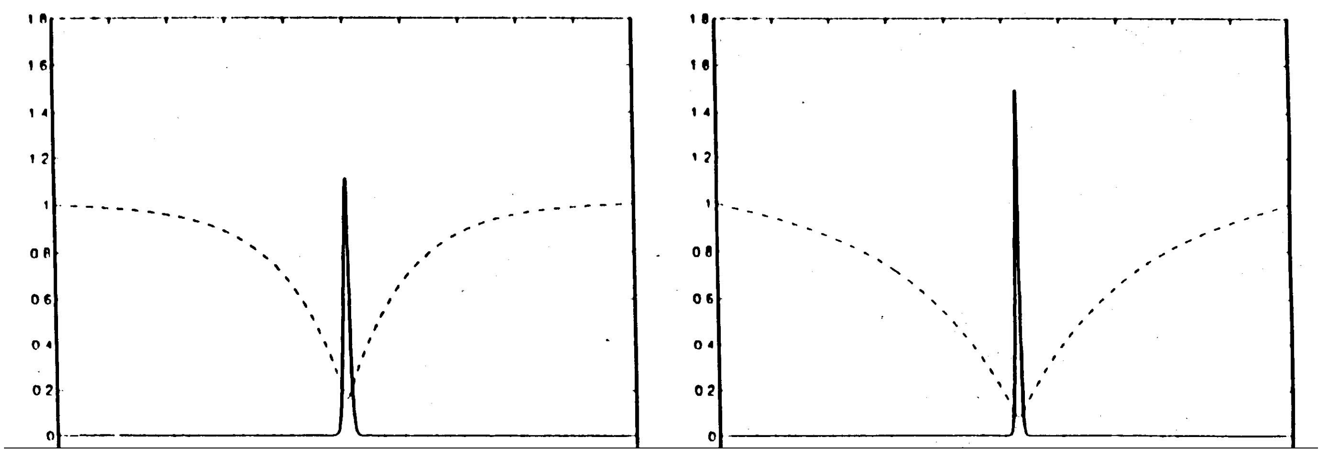
$$\begin{aligned}
\Delta p &= \int_{-\infty}^{\infty} \dot{p} dt \\
&= \epsilon \int_{-\infty}^{\infty} u_0 v_0^2 dt \\
&= \epsilon \frac{6b\sqrt{b}}{u_0} + h.o.t.
\end{aligned}$$

We can use the limits $\pm\infty$ because we linearize around the fast solution, so the contributions to Δp become exponentially small as $|t| \to \infty$ since v_0 becomes exponentially small. A similar calculation shows $\Delta u = O(\epsilon^2)$.

A **stationary 1-pulse** may be created as follows. First observe that the GS model possesses the symmetry $(t, p, q) \to (-t, -p, -q)$. As a result the solution is symmetric in p, so

$$\boxed{\begin{array}{rcll} -\epsilon\sqrt{a} + h.o.t. & = & \frac{1}{2}\epsilon\left(\epsilon^{\sigma}\gamma u_0 - \frac{6b\sqrt{b}}{u_0}\right) + h.o.t. & \text{forward} \\ +\epsilon\sqrt{a} + h.o.t. & = & \frac{1}{2}\epsilon\left(\epsilon^{\sigma}\gamma u_0 + \frac{6b\sqrt{b}}{u_0}\right) + h.o.t. & \text{return} \end{array}}$$

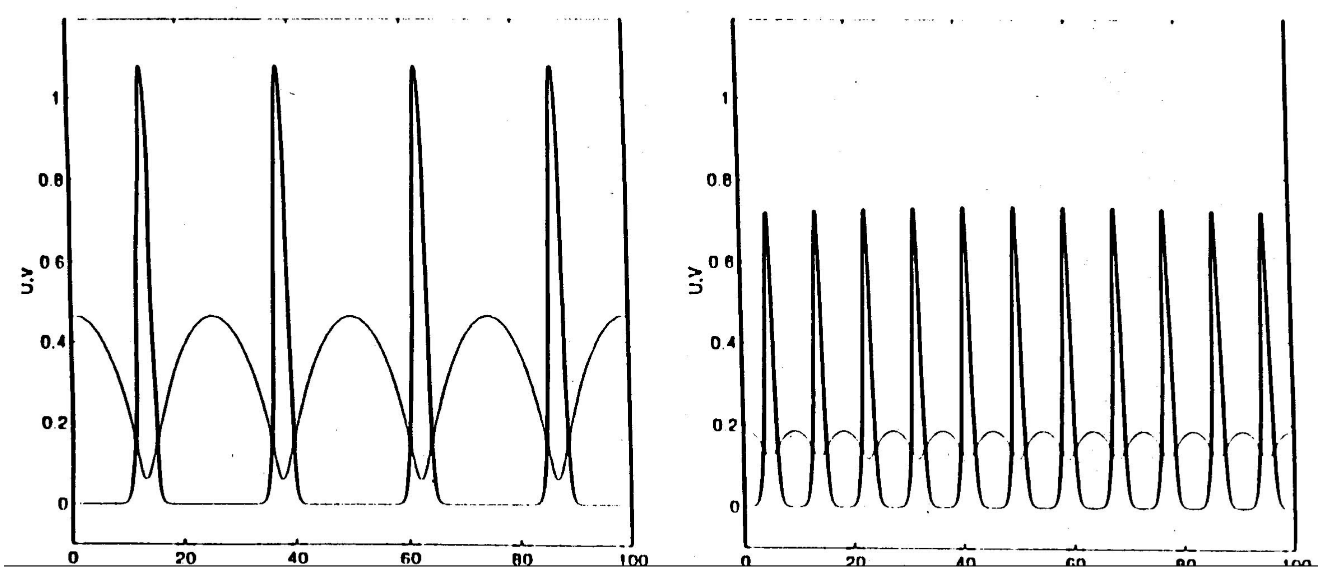
That is, $p_{\text{before takeoff}} = p_{\text{intersection}} - (1/2)\Delta p$, and similarly for $p_{\text{after takeoff}}$. The factor $1/2$ is due to the symmetry of the system. For a stationary pulse set $c \propto \gamma = 0$, subtract the equations above to obtain $u_0^{\pm} = 3b\sqrt{b/a}$ to leading order. This procedure is extended to **stationary N-pulse** orbits by replacing $1/2$ with $N/2$.



Constructing **periodic stationary pulses** is only slightly more difficult, since for $\gamma = 0$ the slow subsystem equations may be solved exactly. Taking the exact solution we may again derive "forward" and "return" conditions and obtain

$$V_{max} = \frac{\sqrt{a(2U_{max} - U_{max}^2)}}{2\sqrt{B}}, \qquad U_{min} = \frac{3B\sqrt{B}}{\sqrt{a(2U_{max} - U_{max}^2)}}$$

Here U, V are scaled back to their original magnitude. Note that as $U_{max} \to 1$, approaching the saddle point, the results of the previous section are recovered.



Now we may try to extend this analysis to **travelling patterns**, i.e. redo the same procedure for $\gamma \neq 0$. As the "forward" and "return" equations derived above show, we must evaluate higher order terms of both the Melnikov function and of $\ell^{U,S}$ in order to determine if the term at order $(1+\sigma)$ can be matched. The analysis shows it cannot, hence in the parameter regime considered **no travelling patterns exist**.

The preceding analysis raises a few questions whose answers (where they are known) would unduly extend this poster. However, some questions you may wish to ask are...

- Are these solutions stable? And hey, where are the N-pulse orbits?
- Is there a multiple scales approach to generating these solutions?
- Numerical experiments seem to suggest travelling waves *do* exist in the considered domain. How does this jibe with the analysis here? (Hint: It involves pulse-splitting.)
- What about 2-D Gray-Scott? Are there any popular articles or, better yet, web sites I can look up to learn more?