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Classification and Stability of Global Inhomogeneous Solutions of a Macroscopic Model of Cell Motion

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Abstract

Many micro-organisms use chemotaxis for aggregation, resulting in stable patterns. In this paper, the amoeba *Dictyostelium discoideum* serves as a model organism for understanding the conditions for aggregation and classification of resulting patterns. To accomplish this, a 1D nonlinear diffusion equation with chemotaxis that models amoeba behavior is analyzed. A classification of the steady state solutions is presented, and a Lyapunov functional is used to determine conditions for stability of inhomogeneous solutions. Changing the chemical sensitivity, production rate of the chemical attractant, or domain length can cause the system to transition from having an asymptotic steady state, to having asymptotically stable single-step solution and multi-stepped stable plateau solutions.

Keywords

Aggregation; Chemotaxis; Inhomogeneous Stability; Lyapunov Functional; Plateau Solutions; *Dictyostelium discoideum*

1. Introduction

As an initial step towards biofilm formation, a wide range of microscopic organisms, including both innocuous amoeba and harmful pathogenic bacteria, are able to use a combination of cell to cell interactions and chemical signals to aggregate into mounds. These mounds are stable structures in the sense that if they are disturbed, the micro-organisms will sense this disturbance and re-form themselves into another mound like structure.

Dictyostelium discoideum is an amoeboid capable of demonstrating fruiting body formation during starvation conditions. The amoeba releases a chemical to signal to other amoebas its location. Using a combination of projecting pseudopodia and hydrostatic pressure, the amoeba is able to orient itself and follow local chemical gradients to find other amoebas [10, 17]. With this procedure, the amoebas are able to aggregate together to form a slug.

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Extensive past work on modeling cell aggregation of amoeba with chemotaxis provided significant insights into the mechanisms for pattern formation due to the emergence of unstable perturbations [3, 8, 9, 13]. However, much of this work implicitly allowed for cells to overlap, and as a result, the models demonstrated blowup when certain conditions were met. Works such as [14, 11] use volume exclusion to implement non-overlapping. In particular, [11] derived a nonlinear diffusion PDE from a stochastic system, describing cells as extended objects with finite volumes and fluctuating membranes.

In this paper, we focus on modeling slug formation using an equation that was derived to model the density of the amoeba under excluded volume conditions [11]:

$$\partial_t u = \nabla \cdot [h(u) \nabla u] - \nabla [g(u) \nabla v] \quad (1)$$

$$\partial_t v = D_c \nabla^2 v + \alpha u - \gamma v. \quad (2)$$

where u and v represent the cell and chemical densities, respectively, and $h(u)$ and $g(u)$ represent cell diffusion and chemotactic rates, respectively. $h(u)$ has a singularity which allows the equation to demonstrate so called fast diffusion, where the diffusion approaches infinity for large enough cell density. It is known that (1–2) demonstrates non-trivial, non-homogeneous patterns, and that a similar 2D equation is capable of demonstrating aggregates, which have been reported to have similar structure to blood vessels [11]. It is also known that linear stability analysis can be used to analyze the stability of the homogeneous steady state under small perturbation, in particular, see Ref. [8].

In this paper, we attempt to analyze the structure and stability of non-homogeneous patterns in a spatially one-dimensional case in order to understand whether or not structures resembling mounds will occur and whether or not they are stable to perturbations. In particular, we establish that multi-stepped patterns will start out unstable, but as the domain becomes larger, oscillatory, non-trivial patterns emerge and, under certain conditions, will become stable. For long enough domains, the stability of the pattern can be characterized by the maximum value of the density profile. Often times, stability can also be determined by whether or not the solutions can be described as spikes or plateaus, as defined in [7] and [8]. Qualitatively, there is no obvious distinction between plateaus and mounds, but it should be noted that the former is a mathematical characterization, and the latter is an observed quality. In our case, we are able to show that for long enough domains, spikes correspond to unstable solutions.

The format of the paper is as follows. In the first section, we examine an example system and perform phase plane analysis to categorize when the constant steady state solution(s) are saddles or centers. Then, we describe the non-homogeneous stationary solutions as a single or multi-stepped patterns using a Hamiltonian framework in a similar manner as [15]. We then use the Hamiltonian to describe how single and multi-stepped solutions bifurcate from a steady state when the steady state is a center. In the following section, we examine the more general system and implement a Lyapunov functional, similar to the one described in [4], to classify several conditions for instability. The existence of a bounded Lyapunov functional says that the solution will converge in time to an asymptotically stable attractor contained in the union of all functions that are local minimum values of the functional. These functions coincide with the stationary solutions. By determining when stationary solutions are not local minima, it is possible to determine which patterns are unstable. Several conditions for instability and stability are established using various inequalities. In particular, we determine the conditions when multi-stepped solutions can be constructed. We establish that each k-step solution, with given parameter values discussed below,

becomes stable or unstable as the domain length approaches infinity. After this, analysis is performed on the general system to indicate when stationary solutions can be classified as plateaus or spikes. In the final section, numerics are performed to show the existence of stable multi-step patterns.

2. Classification of Stationary Solutions

For the rest of the paper, we will derive results for a 1D version of system (1–2). However, many of the results are best expressed by analyzing and examining the specific example from [11],

$$u_t = D \left[\frac{1+u^2}{(1-u)^2} u_x \right]_x - \chi(uv_x)_x \quad (3)$$

$$v_t = D_c v_{xx} - \gamma v + \alpha u \quad (4)$$

on the interval $(0, L)$, $L > 0$, satisfying the boundary conditions

$$u_x(0, t) = v_x(0, t) = u_x(L, t) = v_x(L, t) = 0. \quad (5)$$

In order to do so, we will first introduce a change of variables

$$\rho = u, \Phi = \frac{\gamma}{\alpha} v,$$

$$s = \sqrt{\frac{\gamma}{D_c}} x, \tau = \gamma t,$$

$$\beta = \frac{D}{D_c}, \omega = \frac{\alpha \chi}{\gamma D_c}, \eta = \sqrt{\frac{\gamma}{D_c}} L$$

and consider the system

$$\rho_\tau = \beta \left[\frac{1+\rho^2}{(1-\rho)^2} \rho_s \right]_s - \omega(\rho \Phi_s)_s \quad (6)$$

$$\Phi_\tau = \Phi_{ss} - \Phi + \rho \quad (7)$$

on the interval $(0, \eta)$, $\eta > 0$, satisfying the boundary conditions

$$\rho_s(0, \tau) = \Phi_s(0, \tau) = \rho_s(\eta, \tau) = \Phi_s(\eta, \tau) = 0. \quad (8)$$

Note that if we apply this change of variables to (3–4), we can effectively set $D_c, \alpha, \gamma = 1$ up to some scaling of h and g .

It is shown in [1, 6] that this system admits unique, globally-bounded, nonnegative solutions $\rho, \Phi \in C^{2,1}([0, \eta], [0, \infty))$, for sufficiently smooth initial conditions satisfying compatibility conditions, and these solutions are capable of presenting non-homogeneous

steady state solutions. Under these conditions, ρ is bounded between 0 and 1, and Φ is bounded between 0 and $\max(\|\Phi(s, 0)\|_{L^\infty}, 1)$. We now proceed to characterize the stationary behaviour of the system through a series of manipulations, leading up to a Hamiltonian formulation of the steady state. Thanks to such manipulations, we can express Φ as a function of ρ for stationary solutions.

First we set the left hand side of (6) to zero and integrate from 0 to s to get

$$\beta \frac{1+\rho^2}{(1-\rho)^2} \rho_s = \omega \rho \Phi_s \quad (9)$$

where we set the integration constant to zero in order to satisfy the boundary conditions. Dividing both sides by $\omega \rho(s)$ and then integrating from 0 to s , we get

$$\Phi(s) = \int_0^s \frac{\beta}{\omega} \frac{1+\rho(\zeta)^2}{\rho(\zeta)[1-\rho(\zeta)]^2} \rho \zeta(\zeta) d\zeta + \Phi(0). \quad (10)$$

Evaluating the integral gives the following system for the stationary solutions

$$\Phi = Q(\rho) - K \quad (11)$$

$$\Phi_{ss} = \Phi - \rho \quad (12)$$

where

$$Q(\rho) := \frac{\beta}{\omega} \left[\ln(\rho) + \frac{2}{1-\rho} \right]$$

and

$$K = Q(\rho(0)) - \Phi(0). \quad (13)$$

Let us note that $Q'(\rho) > 0$ for $\rho \in (0, 1)$ with $\mathcal{R}(Q) = (-\infty, \infty)$, so by the Inverse Function Theorem (11) is invertible. For bounded stationary solutions and fixed K , we can define the inverse $f_K: (-\infty, \infty) \rightarrow (0, 1)$. Below for brevity of notation, we will omit the index K and write simply f instead of f_K . For given f , we can define $\rho(\Phi) := f(\Phi)$. $f(\Phi)$ will be used extensively when we define the Hamiltonian for stationary solutions. Also, let us note that if

$$M := \frac{1}{\eta} \int_0^\eta \rho(s) ds, \quad (14)$$

where M is the total cell density and is a conserved quantity with respect to time, then

$$K = \frac{\beta}{\omega \eta} \int_0^\eta \left[\ln(\rho(s)) + \frac{2}{1-\rho(s)} \right] ds - M. \quad (15)$$

As ρ depends on Φ , then we will write $K = K[\Phi]$. In the case when ρ and Φ are constant, we have

$$K = Q(M) - M. \quad (16)$$

2.1. Phase Plane Analysis

To analyze the properties of spatially inhomogeneous steady state solutions, we construct a new system of equations. To do so, we treat $K[\nu]$ as a given constant, substitute $\rho = f(\Phi)$ into (11–12) and set $\psi := \Phi_s$. The stationary solution can then be described with the 2D system of autonomous ODEs:

$$\Phi_s = \psi \quad (17)$$

$$\psi_s = \Phi - f(\Phi) \quad (18)$$

$$\Phi_s(0) = \Phi_s(\eta) = 0. \quad (19)$$

This is a system of Hamiltonian equations with the Hamiltonian

$$H = -\frac{\psi^2}{2} + \frac{1}{2}\Phi^2 - F(\Phi) \quad (20)$$

where $\frac{dF(\Phi)}{d\Phi} = f(\Phi)$. Looking at the Jacobian of the system at a fixed point reveals that the trace is zero, so all fixed points are either saddles or centers.

Alternatively, we can formulate a Hamiltonian in terms of ρ . By substituting $\Phi = Q(\rho) - K$ into (18) and multiplying by $Q(\rho)_s$ to get

$$0 = Q(\rho)_{ss}Q(\rho)_s - Q(\rho)_sQ(\rho) + KQ(\rho)_s + Q(\rho)_s\rho$$

and taking the integral with respect to ρ gives

$$\tilde{H} = \frac{Q(\rho)_s^2}{2} - \frac{Q(\rho)^2}{2} + KQ(\rho) - B(\rho) + Q(\rho)\rho \quad (21)$$

where $B(\rho)$ is the integral of $Q(\rho)$:

$$B(\rho) := \frac{\beta}{\omega} [\rho \ln(\rho) - \rho - 2 \ln(1 - \rho)] \quad (22)$$

The system (17–19) has fixed points $(\Phi, \psi) = (f(\Phi), 0)$ and its dynamics depend not only on the parameters, but also on the value of $K[\Phi]$. Since $Q(\rho) - K: [0, 1] \rightarrow [-\infty, \infty]$ is monotonically increasing, the inverse, $f(\Phi)$, is defined and sigmoid in shape with asymptotes $f(-\infty) = 0$ and $f(\infty) = 1$.

Typically, the equation $\Phi = f(\Phi)$ has either one or three roots, Φ_i , which correspond to fixed points S_i of system (17–18). This can be observed by numerically solving for solutions to the PDE system (see numerics section below) and examining resulting steady states. If we solve the PDE and look the resulting steady states with $M = 0.25$, $\eta = 40$, $\beta = 0.1$, and $\omega = 0.7$, and compare it to the results with $\omega = 1$, using initial conditions described in the numerics section, it is possible to see that the former converges to a constant steady state solution, while the latter results in an inhomogeneous solution. In particular, the former approaches a steady state solution with $(\rho(\eta), \Phi(\eta)) = (0.25, 0.25)$ and the latter with $(\rho(\eta), \Phi(\eta)) = (0.0499, 0.0499)$. Using (13) and the definition of f we can examine how many

roots exist for $f(\Phi) - \Phi$ for these two choices of solutions (see Figure 1). The Φ_i generally have to be numerically solved for in order to determine their values. This can be accomplished by inverting f back and solving $Q(\Phi) - K = \Phi$ (see numerics section below for an example of this).

Lemma 2.1. If (17–18) has a single fixed point, it is a saddle. If it has three fixed points with $\Phi_1 < \Phi_2 < \Phi_3$, then Φ_2 is a center and the other two fixed points are saddles.

Proof. Taking the trace and determinant of the Jacobian of the system, we see the eigenvalues, $\nu_{\pm}$, of the fixed points can be determined from the equations

$$\nu_+ + \nu_- = 0 \quad (23)$$

$$\nu_+ \nu_- = f'(\Phi_i) - 1. \quad (24)$$

Consider a fixed point Φ_i . If $f'(\Phi_i) < 1$, then the fixed point is a saddle. If $f'(\Phi_i) > 1$, then the fixed point is a center. Note that if we have $f'(\Phi_i) > 1$, then, at Φ_i , we can use the fact that $f(\Phi) - \Phi$ is increasing and the asymptotic behaviour of $f(\Phi)$ to deduce that there are saddles, Φ_1 and Φ_3 , such that $\Phi_1 < \Phi_i < \Phi_3$. In other words, in the case of one root, we must always have a saddle. If we have three roots, we have a center along with two saddles, since the slope of the middle root is larger than the slope of the line (see Figure 1b).

As will be seen later, inhomogeneous patterns can only occur if we have a center, so we will consider the case where we have three roots, $\Phi_1 < \Phi_2 < \Phi_3$.

2.2. Hamiltonian Characterization

Additional information about the structure of the steady state solutions of (17–19) can be gained by examining the Hamiltonian (20). In particular, since the Hamiltonian is independent of s -variable, for fixed Hamiltonian constant H , we can examine the Hamiltonian curves and solve for ψ as a function of Φ to get

$$\psi = \pm \sqrt{2 \left(-F(\Phi) + \frac{\Phi^2}{2} - H \right)}. \quad (25)$$

The plus and minus signs correspond to the positive and negative solutions for ψ . It is also seen that Φ is symmetric across the $\psi = 0$ axis, and we are free to choose which sign we examine. See figure 2 for sample Hamiltonian curves with $\omega = 10$, $\beta = 1$, and $K = -0.1392$. In this case (Φ_1, Φ_2, Φ_3) is approximately equal to $(0.05, 0.318, 0.625)$.

Unless otherwise specified, from this point forward, we only consider the positive part of the curve where $\psi \geq 0$. In this case, with $\psi = \Phi_s$, we can solve for s as a function of Φ along the positive curve by inverting both sides of equation (25) and integrating with respect to Φ . Doing this we get

$$s = \int_{\Phi(0)}^{\Phi(s)} \frac{d\Phi}{\sqrt{2 \left(-F(\Phi) + \frac{\Phi^2}{2} - H \right)}}. \quad (26)$$

(26) describes the s -location where the specified Φ occurs with given Hamiltonian energy H .

The authors would like to note at this time that equations (25, 26) are only currently known to be well defined and real for a given non-constant stationary solution, $(\Phi(s), \psi(s))$. If H or

$\Phi(0)$ are chosen arbitrarily, then the value inside the square-root (25) may become negative, and (26) will no longer be real, if defined at all.

The minimal and maximal values of Φ , $\Phi_{\min}$ and $\Phi_{\max}$, occur at the turning points of the Hamiltonian, when $\psi = 0$, i.e., can be found from the equality:

$$0 = -F(\Phi) + \frac{\Phi^2}{2} - H. \quad (27)$$

If we instead use the alternate Hamiltonian, $\tilde{H}$, we can use the chain rule and similarly solve for

$$s = \int_{\rho(0)}^{\rho(s)} \frac{Q'(\rho) d\rho}{\sqrt{2(\tilde{H} + (Q(\rho)^2/2 - KQ(\rho)) + (B(\rho) - \rho Q(\rho)))}}, \quad (28)$$

where we use the fact that $Q'(\rho) > 0$ on the domain, and the minimal and maximal values of ρ occur at the turning points, when the denominator evaluates to 0.

If we use $\Phi_{\min}$ and $\Phi_{\max}$ (obtained by solving (27)) as parameters, then the duration of the half curve's orbit, $\tau(\Phi_{\min})$, satisfies

$$\mathcal{T} = \int_{\Phi_{\min}}^{\Phi_{\max}} \frac{d\Phi}{\sqrt{2(-F(\Phi) + F(\Phi_{\min}) + \frac{\Phi^2 - \Phi_{\min}^2}{2})}} \quad (29)$$

Duration will become important as we link solutions to the Hamiltonian equation to solutions satisfying the boundary value problem of (17–19).

These results can be put in a more concrete form with the following Theorem.

Theorem 2.2. For any given $\rho(0) > 0$, and $\Phi(0) > 0$, $f(\Phi) \in C^1([-\infty, \infty])$ is well defined and $F(\Phi) \in C^2([-\infty, \infty])$ is defined up to a constant. Assuming that the equation $f(\Phi) - \Phi = 0$ has three distinct roots, Φ_1 , Φ_2 , and Φ_3 , and that the constant H can be chosen in such a way that Eq.(27) has positive roots $\Phi_{\min}, \Phi_{\max}$ satisfying $\Phi_1 < \Phi_{\min} < \Phi_2 < \Phi_{\max} < \Phi_3$. Then:

1. It is possible to define $\tilde{\psi}(\Phi) \in C^2((\Phi_{\min}, \Phi_{\max}))$ by (25) and $\Phi(s) \in C^2((0, \eta))$ implicitly by (26).
2. For $\psi(s) = \tilde{\psi}(\Phi(s))$, $(\Phi(s), \psi(s))$ are non-homogenous single-step solutions to the ODE described in (17–18) and there is a unique $\mathcal{T}$ such that $(\Phi(s), \psi(s))$ also satisfy the boundary conditions described in (19) using the chosen domain length $\eta = \mathcal{T}$.
3. We can define $\rho(s) = f(\Phi(s))$ to get step-like solutions $(\rho(s), \Phi(s))$ that are unique steady state solutions to (6), (7) satisfying boundary conditions (8) with the specified $\mathcal{T}$.
4. The reflection (ρ, Φ) over the domain is also a steady state solution to (6), (7) that satisfies the boundary conditions (8) with the specified $\mathcal{T}$.

Proof. Given $(\rho(0), \Phi(0))$, we define K using (13). Having K , it is possible to define $f(\Phi)$ as the inverse of (11) by the inverse function Theorem. Since $f(\Phi)$ is C^1 class, the indefinite integral $F(\Phi)$ is well defined up to a constant of integration and is C^2 class.

We can assume without loss of generality that $\Phi_{\min} := \Phi(0)$. Using the assumption that $f(\Phi) - \Phi$ has three roots, and the fact that $f(-\infty) = 0$, $f(\infty) = 1$, we have,

$$f(\Phi) - \Phi < 0 \text{ for } \Phi \in (\Phi_1, \Phi_2)$$

$$f(\Phi) - \Phi > 0 \text{ for } \Phi \in (\Phi_2, \Phi_3)$$

Integrating the function $f(\Phi) - \Phi$ with respect to Φ and defining H using (27), we see that it is possible to define $\tilde{\psi}: (\Phi_{\min}, \Phi_{\max}) \rightarrow \mathbb{R}_+$ by choosing the positive sign in (25). Also, from the above statements, it follows the $\tilde{\psi}$ is C^2 class in $(\Phi_{\min}, \Phi_{\max})$.

Since $\tilde{\psi} \geq 0$ for $\Phi \in (\Phi_{\min}, \Phi_{\max})$, we can define, using (26), a function $s(\Phi)$, with domain $\mathcal{D}(s) = (\Phi_{\min}, \Phi_{\max})$ and range $\mathcal{R}(s) = (0, s(\Phi_{\max}))$. $s(\Phi)$ is well defined since for $\Phi_{\min} < \Phi < \infty$ we have some constant $\tilde{C} > 0$ such that:

$$s = \int_{\Phi_{\min}}^{\Phi} \frac{d\Phi}{\sqrt{2(-F(\Phi) + \frac{\Phi^2}{2} - H)}} \quad (30)$$

$$\leq \int_{\Phi_{\min}}^{\Phi} \frac{d\Phi}{\sqrt{\tilde{C}(\Phi - \Phi_{\min})(\Phi_{\max} - \Phi)}} < \infty. \quad (31)$$

Note that the second line follows from the fact that the roots of $-F(\Phi) + \frac{\Phi^2}{2} - H$ at $\Phi_{\min}$ and $\Phi_{\max}$ are simple. The derivative of this function is $-f(\Phi) + \Phi$, which by the above statements and assumptions is not zero at the roots because $\Phi_{\min}, \Phi_{\max} \in \Phi_1, \Phi_2, \Phi_3$. Otherwise, our trajectory would be a fixed point or tend to a fixed point.

Since $s(\Phi)$ is monotonically increasing, it has a monotonically increasing inverse $\Phi(s)$. This establishes part 1.

Using part 1, we can now define the pull back $\psi(s) := \tilde{\psi}(\Phi(s))$. By computing the derivative of s_Φ by means of (26) and inverting it, it is straightforward to see that

$$\frac{d\Phi(s)}{ds} = \psi(s).$$

Furthermore, taking the derivative of both sides of (25) (with 'plus' sign) we get that ψ satisfies (18). Since $\Phi_{\max} < \infty$, there is a unique $\mathcal{T}$ such that $\Phi(\mathcal{T}) = \Phi_{\max}$. In this case

$$\tilde{\psi}(\Phi_{\min}) = \tilde{\psi}(\Phi_{\max}) = 0$$

and

$$\Phi_{\min} = \Phi(0) \text{ with } \Phi_{\max} = \Phi(\eta)$$

satisfying the boundary conditions.

Part 3 follows from the fact that we can define $\rho(s) = f(\Phi(s))$, and taking the derivative of $\rho(s)$ gives

$$\rho_s = f'(\Phi) \Phi_s = \frac{\omega}{\beta} \left(\frac{\rho(1-\rho)^2}{1+\rho^2} \right) \Phi_s.$$

This equation is equivalent to (9) which we can take the derivative of to get (6) with $\rho_\tau = 0$ and (7) follows from part 2. The boundary conditions for ρ are satisfied using (9) and are satisfied for Φ by part 2. Uniqueness follows from [1], establishing part 3.

Using a change of variables, $s \rightarrow -s + \eta$, it is possible to see that the reflection of the solution across the domain also satisfies the stationary equation to (6), (7) with the caveat that ψ changes sign. This yields part 4.

Remark 2.3. If $\Phi_{\min}$ or $\Phi_{\max}$ equals either Φ_1 , Φ_2 , or Φ_3 , then it is instead possible to define $\Phi(s)$ as the appropriate constant function, $\rho = \Phi$, and $\psi = 0$ which satisfies the conditions of being a stationary solution.

Corollary 2.4. All positive non-homogenous steady state solutions to (6) satisfying boundary conditions (8) are a sequence of single-steps alternating between specific values of $\Phi_{\min}$ and $\Phi_{\max}$.

Proof. Given a positive non-homogenous bounded solution $(\rho(s), \Phi(s))$, let $s_1 > 0$ be the first point after $s = 0$ where either $\rho_s = 0$. If $\rho_s = 0$, then $\Phi_s = 0$ where the latter result is ruled out by positivity. We can therefore restrict the domain to $[0, s_1]$ with $(\rho(s), \Phi(s))$ as the unique step solution to the restricted boundary value problem. At this point, we see from the Hamiltonian dynamics given in the phase plane analysis that having a non-constant steady state solution means that $f(\Phi) - \Phi$ is sigmoid with three roots. In order to satisfy the boundary conditions, $\psi(\Phi)$ must have two roots. By the above Theorem, since we have $K = Q(\rho(0)) - \Phi(0)$, and by uniqueness, we must have $\Phi(s_1)$ either be $\Phi_{\max}$ or $\Phi_{\min}$. In either case, if $s_1 = \eta$, we are done. Otherwise, we can repeat the argument for the next critical point, s_2 . Notice that K stays the same for the restricted solution with domain $[s_1, s_2]$, since K is an integration constant with $K = Q(\rho(s)) - \Phi(s)$, and s_1 is in both the first and second domains. Furthermore, since K stays the same, we have the same $\Phi_{\min}$ and $\Phi_{\max}$, and their corresponding ρ values are also the same. By part 4 of the Theorem and uniqueness, the second step must be a reflection of the previous step because the steps share the same minimum, maximum, and K value. Also note that because it is a reflection, the second step has the same step length as the first step with $s_2 = s_1 + \mathcal{T}$. Repeating this argument until $s_n = \eta$, for some $\eta > 0$, gives $\mathcal{T}$ divides η , and the steps must alternate between reflections of the first step.

2.3. Generation of Multi-Stepped Solutions

To get spatially non-homogenous solutions along the center manifold that corresponds to stationary solution of (6), we need the trajectory to begin and end at $\psi = 0$ after duration η by the boundary conditions $\psi(0) = \psi(\eta) = 0$. Note that this condition cannot be satisfied if we only had a single saddle as a fixed point. Using the symmetry of Φ across the ψ -axis, it is possible to see that following the (Φ, ψ) trajectory curves gives the condition $\eta = k\mathcal{T}$ for some integer k . To parametrize possible curves, let us vary the point of intersection on the ψ -axis, $(\Phi_{\max}, 0)$, where $\Phi_2 < \Phi_{\max} < \Phi_3$ and let $\mathcal{T}$ be the duration of the half curve's orbit that ends at $(\Phi_{\max}, 0)$. As $\Phi_{\max}$ increases, the curves move away from the fixed point. Eventually we will approach either a heteroclinic orbit connecting S_1 and S_3 or a homoclinic

orbit connecting one of the roots to itself. Using (27), it may or may not be possible to solve for $\Phi = \Phi_1$ such that

$$0 = F(\Phi) - \frac{\Phi^2}{2} - F(\Phi_1) + \frac{\Phi_1^2}{2}.$$

If no such Φ exists, then the Hamiltonian curve containing S_1 does not connect back to the ψ -axis, which occurs when S_3 has a homoclinic orbit connecting to itself. If such a Φ exists, then we either have a heteroclinic orbit, with $\Phi = \Phi_3$, or a homoclinic orbit connecting S_1 to itself with $\Phi < \Phi_3$. In all of these cases, for large enough $\Phi_{\max}$, the duration for the half curve's orbit approaches ∞ .

We now calculate how the duration behaves as $\Phi_{\max}$ approaches Φ_2 from above, ($\Phi_{\max} \searrow \Phi_2$). The periodic solution is non-homogeneous, but its variation tends to zero, that is to say $\max_s \Phi(s) - \min_s \Phi(s) \rightarrow 0$ and $|\Phi(s) - \Phi_2| \rightarrow 0$ for all $s \in (-\infty, \infty)$. By using (11) we conclude that $|\rho(s) - \rho_2| \rightarrow 0$ for all $s \in (-\infty, \infty)$ with $\rho_2 = \Phi_2$. Hence by (12), we infer that $\Phi_{ss}(s) \rightarrow 0$, and consequently that $\Phi_s(s) \rightarrow 0$ for all $s \in (-\infty, \infty)$. Knowing this, we can approximate the solution by the solution of the linearization of system (17–18) around $(\Phi, \psi) = S_2$. Solving the linearized system yields that the Φ is periodic with half-period $\mathcal{T}^*$ if

$\mathcal{T}^*|\nu_+| = \mathcal{T}^*|\nu_-| = \pi$, where ν_+ and $\nu_- = -\nu_+$ with $\nu_+ = i\sqrt{f'(\Phi_2) - 1}$ are the strictly imaginary eigenvalues of the Jacobian of (17–18) at point S_2 . This gives us the limiting duration

$$\lim_{\Phi_{\max} \searrow \Phi_2} \mathcal{T}(\Phi_{\max}) = \mathcal{T}^* = \frac{\pi}{\sqrt{f'(\Phi_2) - 1}}. \quad (32)$$

We will later show that given a domain of length $\eta < \mathcal{T}^*$, there is at least one non-homogeneous solution. For $\eta < \mathcal{T}^*$, we cannot rule out the possibility of non-homogeneous solutions existing, as we cannot establish the monotonicity of $\mathcal{T}(\Phi_{\min})$.

In order to describe the generation of multi-step solutions, we first recall that $\eta = k\mathcal{T}$, where k is the number of half cycles, or steps, the solution contains. Multi-stepped stationary solutions of (17–19) for $k \geq 1$ can only exist with duration, $\mathcal{T} = \eta/k$. So the generation of new stationary solutions corresponds to when the first inhomogeneous solution of (17–19) with domain length $k\mathcal{T}$ appears. This is equivalent to satisfying the linearized condition

$$\mathcal{T}^* = \eta/k = \frac{\pi}{\sqrt{f'(\Phi_2) - 1}}.$$

This process of bifurcating new periodic solutions due to changes in domain length relates to the generation of new eigenvalues of an elliptic operator. For further information on branching solutions, see Ref. [5].

In general, $f'(\Phi_2)$ is hard to determine since we have to solve for Φ_2 . However, for the constant solution, $\Phi = \tilde{M}$, we recall that $\mathcal{K}(\Phi)$ defines the inverse with respect to ρ . According to (11), we have

$$f'(\Phi_2) = \frac{\omega}{\beta} \left[\frac{\tilde{M}(1 - \tilde{M})^2}{1 + \tilde{M}^2} \right] \quad (33)$$

where $\tilde{M}$ satisfies $0 = Q(\tilde{M}) - \tilde{M} - K$ from (16).

We now use the chemotactic strength, ω , as a parameter and the fact that in the limit of zero amplitude oscillations we can substitute (33) into (32) to get the following result

Lemma 2.5. Assuming the same conditions as Theorem 2.2, a k -step stationary solution to (6) exists for $\omega > \omega_k$ when

$$\omega_k = \frac{\beta(1 + \tilde{M}^2) \left(\left(\frac{k\pi}{\eta} \right)^2 + 1 \right)}{\tilde{M}(1 - \tilde{M})^2}. \quad (34)$$

Proof. Recall that by the assumptions, the system (17–18) is Hamiltonian with a center and two saddles. The phase plane contains Hamiltonian curves that connect the $\psi = 0$ axis to itself. By the above calculation in (32), there are orbits whose duration is arbitrarily close to the duration $\mathcal{T}^*$ for given ω and since there is either an orbit homoclinic to the point S_1 or S_3 or a heteroclinic orbit connecting S_1 with S_3 . Both kinds of orbits have infinite duration. The function (29) is continuous with respect to $\Phi_{\min} \in (\Phi_1, \Phi_2)$ due to the continuity of the integrand. So, for any duration $\mathcal{T} \in (\mathcal{T}^*, \infty)$, there exists at least one corresponding Hamiltonian curve whose orbit has that duration. Since each Hamiltonian curve satisfies the boundary conditions for some domain length η , it remains to show there is a duration $\mathcal{T}_k = \eta/k > \mathcal{T}^*$ for there to exist a k -step solution on domain length L . Let $\omega = \omega_k + R$, $R > 0$, and using (32), (33), and $f'(\Phi_2) > 0$ we have,

$$\begin{aligned} \mathcal{T}^* &= \frac{\pi}{\sqrt{f'(v_2) - 1}} \\ &= \frac{\pi}{\sqrt{\left(\frac{k\pi}{\eta} \right)^2 + Rf'(\Phi_2)}} \\ &< \frac{\pi}{\sqrt{\left(\frac{k\pi}{\eta} \right)^2}} \\ &= \eta/k = \mathcal{T}_k \end{aligned}$$

We note that there is a unique correspondence between our choice of K and the value of $\tilde{M}$ since $\tilde{M} = \Phi_2$. This correspondence allows us to switch the roles of $\tilde{M}$ and K , making $\tilde{M}$ a parameter for determining the dynamics of the system.

Notice that (34) can also be used to count the number of stationary solutions that the given parameters can produce. Given $\omega_k < \omega < \omega_{k+1}$, there are k known curves that satisfy the conditions for the given $\tilde{M}$. However, if we were to try and leave $\tilde{M}$ arbitrary, then we cannot, at this time, discount the possibility for multiple k -step solutions with the same value of $\tilde{M}$.

3. Stability Analysis of Solutions

3.1. Lyapunov Stability Condition

In order to analyze the stability of multiple stepped equations, we will define a Lyapunov functional and describe the conditions when the stationary solutions are local minimums. Here we consider the system

$$\rho_\tau = (h(\rho)\rho_s)_s - (g(\rho)\Phi_s)_s \quad (35)$$

$$\Phi_\tau = \Phi_{ss} - \Phi + \rho \quad (36)$$

$$\rho_s(0) = \Phi_s(0) = \rho_s(\eta) = \Phi_s(\eta) = 0. \quad (37)$$

We define a generalized entropic functional

$$S = - \int_0^\eta C(\rho(x)) dx \quad (38)$$

where $C(\rho)$ is the convex function determined by the equality:

$$C''(\rho) = \frac{h(\rho)}{g(\rho)}. \quad (39)$$

Let us note that the function $C(\cdot)$ is defined only up to a term $c_1\rho + c_2$. However, integration of this term over space gives a constant independent of τ , due to the mass conservation $(\eta)^{-1} \int_0^\eta \rho(s, \tau) ds = M$. For definiteness, we will take $c_1 = c_2 = 0$ here. Let us also define the generalized free energy

$$F = \int_0^\eta \frac{1}{2}(\Phi_s)^2 ds + \int_0^\eta \frac{1}{2}\Phi^2 ds - \int_0^\eta \rho\Phi ds + \int_0^\eta C(\rho) ds. \quad (40)$$

Theorem 3.1. If $\rho \in (\rho_{\min}, \rho_{\max})$, where $0 < \rho_{\min} < \rho_{\max}$, $g(\rho) > 0$, $h(\rho) \geq 0$, and $\Phi \geq 0$. Then F is bounded below and is a Lyapunov functional for the system (35–36).

Proof. Since $\rho_{\min} < \rho < \rho_{\max}$, it follows that $\frac{1}{2}\Phi^2 - \rho\Phi$ reaches a critical point with respect to Φ at $-\frac{1}{2}\rho^2$ when $\Phi = \rho$. This critical point is a minimum since the second derivative yields $1 > 0$.

Since $C''(\rho) \geq 0$, it follows that $C(\rho) \geq 0$. As a consequence, the functional is bounded below by

$$F(\rho) \geq - \int_0^\eta \frac{1}{2}\rho^2 ds \quad (41)$$

$$\geq - \frac{\eta}{2}\rho_{\max}^2 \quad (42)$$

Note that for (6–7), the functional is bounded below by $-\frac{\eta}{2}$ since $\rho < 1$.

Taking the time derivative, it is possible to show that for non-stationary ρ and Φ , the free energy

$$F = \int_0^\eta \frac{1}{2}(\Phi_s)^2 ds + \int_0^\eta \frac{1}{2}\Phi^2 ds - \int_0^\eta \rho\Phi ds + \int_0^\eta C(\rho) ds$$

is decreasing with respect to time.

$$\frac{dF}{d\tau} = \int_0^\eta \Phi_s \Phi_{\tau s} ds + \int_0^\eta \Phi \Phi_\tau ds - \int_0^\eta \rho_\tau \Phi - \rho \Phi_\tau ds + \int_0^\eta C'(\rho) \rho_\tau ds \quad (43)$$

$$= \int_0^\eta (-\Phi_{ss} + \Phi + \rho) \Phi_\tau ds + \int_0^\eta (-\Phi + C'(\rho)) \rho_\tau ds \quad (44)$$

$$= - \int_0^\eta \Phi_\tau^2 ds + \int_0^\eta (-\Phi + C'(\rho)) (h(\rho) \rho_s - g(\rho) \Phi_s) ds \quad (45)$$

$$= - \int_0^\eta \Phi_\tau^2 ds - \int_0^\eta (-\Phi_s + C''(\rho) \rho_s) (h(\rho) \rho_s + g(\rho) \Phi_s) ds \quad (46)$$

$$= - \int_0^\eta \Phi_\tau^2 ds - \int_0^\eta g(\rho) (-\Phi_s + C''(\rho) \rho_s)^2 ds \quad (47)$$

$$\leq 0 \quad (48)$$

where we used integration by parts and the no-flux boundary conditions to get the second and fourth lines, and substitution with (35) to get the third line. The last line follows from the positivity of $g(\rho)$. Notice that $\dot{F} = 0$ if and only if $\Phi_\tau = 0$ and $-g(\rho)\Phi_s + h(\rho)\rho_s = 0$. The latter condition implies $\rho_\tau = 0$. If $\rho_\tau = 0$ we have that $-g(\rho)\Phi_s + h(\rho)\rho_s = \text{const.}$ and by boundary conditions, we must have the constant be zero. $\dot{F} < 0$ if and only if the (ρ, Φ) are not stationary solutions.

This forms an H-Theorem in the canonical ensemble. The free energy is always decreasing and it is bounded below, its minimums correspond to stationary solutions. Moreover, the existence of this functional indicates that over time, the solutions will converge to one of these stationary solutions.

In order to determine the stability of the minimum values of the functional F , we look at the first and second variational derivatives. Taking the first and second variational derivatives of F gives

$$\delta F = \int_0^\eta \Phi_s \delta \Phi_s ds + \int_0^\eta \Phi \delta \Phi ds - \int_0^\eta \rho \delta \Phi ds - \int_0^\eta \delta \rho \Phi ds + \int_0^\eta C'(\rho) \delta \rho ds \quad (49)$$

$$\delta^2 F = \int_0^\eta (\delta \Phi_s)^2 ds + \int_0^\eta (\delta \Phi)^2 ds - 2 \int_0^\eta \delta \rho \delta \Phi ds + \int_0^\eta C''(\rho) (\delta \rho)^2 ds. \quad (50)$$

If we find a perturbation $\delta \rho$ and $\delta \Phi$ such that at a fixed point, $\delta^2 F(\delta \rho, \delta \Phi) > 0$, then the fixed point is unstable under this perturbation. With this goal in mind, we consider perturbations that preserve the total amount of chemical density and that satisfy the boundary conditions. Assuming that

$$\delta \rho(s) = \sum_{k>0} A_k \cos(k\pi s/\eta) \quad (51)$$

$$\delta \Phi(s) = \sum_{l>0} C_l \cos(l\pi s/\eta), \quad (52)$$

it is possible to see

$$\int_0^\eta (\delta\Phi_s)^2 ds = \frac{\eta}{2} \sum_{l>0} \mu_l^2 C_l^2 \quad (53)$$

$$\int_0^\eta (\delta\Phi)^2 ds = \frac{\eta}{2} \sum_{l>0} C_l^2 \quad (54)$$

$$-2 \int_0^\eta \delta\rho \delta\Phi dx = - \sum_{l,k>0} \delta_{k,l} \eta A_k C_k, \quad (55)$$

where $\delta_{k,l}$ is the Kronecker delta and $\mu_k = \left(\frac{\pi k}{\eta}\right)$. So $(\delta^2 F)(\delta\rho, \delta\Phi) < 0$ when

$$0 > \frac{1}{\eta} \int_0^\eta \left(\sum_{k>0} A_k \cos(\mu_k s) \right)^2 C'' ds - \sum_{k,l>0} A_k C_l \delta_{k,l} + \sum_{l>0} \left(\frac{\mu_l^2}{2} + \frac{1}{2} \right) C_l^2. \quad (56)$$

Since A_k and C_l are constant for given perturbation, we can minimize the right hand side of the equation with respect to each C_l . This has the effect of choosing the most unstable choice of $\delta\Phi$ for given choice of $\delta\rho$. The critical points that occur must be minimums since evaluating the second derivative with respect to an arbitrary C_l yields

$$\mu_l^2 + 1 > 0.$$

Therefore, the minimums occur when

$$- \sum_{k>0} A_k \delta_{k,l} + (\mu_l^2 + 1) C_l = 0$$

or

$$C_l = \frac{A_l}{\mu_l^2 + 1}.$$

Substituting this choice of C_l in for the unstable case gives

$$0 > \frac{1}{\eta} \int_0^\eta (\delta\rho)^2 C'' ds - \sum_{k>0} \frac{A_k^2}{\mu_k^2 + 1} + \sum_{k>0} \frac{A_k^2}{2(\mu_k^2 + 1)} \quad (57)$$

$$= \frac{1}{\eta} \int_0^\eta (\delta\rho)^2 C'' ds - \sum_{k>0} \frac{A_k^2}{2(\mu_k^2 + 1)}. \quad (58)$$

If instability will occur for the prescribed perturbations, it will occur when the stationary solution satisfies the general instability condition

$$\int_0^\eta C''(\rho(s)) \delta \rho(s)^2 ds < \sum_{k>0} \frac{A_k^2 \eta}{2(\mu_k^2 + 1)}. \quad (59)$$

Since the instability condition holds if and only if the prescribed perturbation is unstable with respect to the stationary solution, if for any concentration preserving perturbation that is the limit of sums of cosines, i.e., functions in $L^2([0, \eta])$ with zero mean that satisfy the boundary conditions, we have

$$0 \leq \sup_{\delta \rho} \sum_{k>0} \frac{A_k^2 \eta}{2(\mu_k^2 + 1)} - \int_0^\eta C''(\rho(s)) \delta \rho^2 ds, \quad (60)$$

then the stationary solution is stable.

This condition is equivalent to all $n \times n$ matrices of the form

$$\mathcal{R} - \mathcal{Q}$$

having non-positive eigenvalues, where $\mathcal{R}$ is a diagonal matrix with

$$\mathcal{R}_{ii} = \frac{\eta}{2(\mu_i^2 + 1)}$$

and

$$\mathcal{Q}_{i,j} = \int_0^\eta C''(\rho(s)) \cos(\mu_i s) \cos(\mu_j s) ds.$$

In general, it seems that this expression has to be evaluated numerically in order to determine the stability of the solution. However, we can state a few estimates about this equation. If we choose $A_1 = 1$ and $A_k = 0$ for $k \neq 1$, then using Holder's inequality we see instability will occur if

$$\|C''\|_{L^\infty} < \frac{1}{\left(\frac{\pi}{\eta}\right)^2 + 1}. \quad (61)$$

For the stability condition, we note that

$$\sup_{\delta \rho} \sum_{k>0} A_k^2 \frac{\eta}{2(\mu_k^2 + 1)} - \int_0^\eta C''(\rho(s)) \delta \rho^2 ds$$

$$\leq \sup_{\delta \rho} \sum_{k>0} A_k^2 \frac{\eta}{2(\mu_1^2 + 1)} - \int_0^\eta C''(\rho(s)) \delta \rho^2 ds \quad (62)$$

$$\leq \sup_{\delta \rho} \frac{\eta}{2(\mu_1^2 + 1)} \sum_{k>0} A_k^2 - \int_0^\eta C''(\rho(s)) \delta \rho^2 ds \quad (63)$$

$$\leq \sup_{\delta\rho} \frac{1}{\mu_1^2 + 1} \|\delta\rho\|_{L^2}^2 - \int_0^\eta C''(\rho(s)) \delta\rho^2 ds \quad (64)$$

$$\leq \sup_{\delta\rho} \frac{1}{\mu_1^2 + 1} \|\delta\rho\|_{L^2}^2 - \inf C''(\rho(s)) \int_0^\eta \delta\rho^2 ds \quad (65)$$

$$\leq \sup_{\delta\rho} \|\delta\rho\|_{L^2}^2 \left[\frac{1}{\mu_1^2 + 1} - \inf C''(\rho(s)) \right] \quad (66)$$

where the first inequality follows from $\mu_k > \mu_1$, and the third and fifth lines from the observation that

$$\|\delta\rho\|_{L^2}^2 = \int_0^\eta \delta\rho^2 ds = \int_0^\eta \left(\sum_{k>0} A_k \cos(\mu_k s) \right)^2 ds = \frac{\eta}{2} \sum_{k>0} A_k^2.$$

Using (66) and (60), we have stability if

$$\frac{1}{\mu_1^2 + 1} < \inf_s C''(\rho(s)) \quad (67)$$

These results lead to the following Theorem.

Theorem 3.2. Assuming the hypothesis found in Theorem 3.1, stationary solutions to the system (35–36) are stable if they satisfy

$$\inf C'' \geq \frac{1}{\left(\frac{\pi}{\eta}\right)^2 + 1} \quad (68)$$

and are unstable if

$$\|C''\|_{L^\infty} < \frac{1}{\left(\frac{\pi}{\eta}\right)^2 + 1}. \quad (69)$$

Notice that inequality (68) is in agreement with the linear stability condition, which can be obtained by computing the eigenvalues of the linearization matrix by assuming the perturbations of the components of the solution $(M, \bar{M})$ proportional to $\cos(\mu_1 x)$ (see Ref.

[2], [12]). These eigenvalues are non-positive if and only if $\frac{h(M)}{g(M)} \geq \frac{1}{\left(\frac{\pi}{\eta}\right)^2 + 1}$. If this condition does not hold (for example, for large $g(M)$, which corresponds to large ω in the case of system (3, 4)), a bifurcation occurs and the constant solution becomes unstable, converging in time towards an inhomogeneous steady state solution. In particular, the constant solution $(M, \bar{M})$ is linearly unstable for the perturbations $\cos(\mu_k x)$, if

$$\frac{h(M)}{g(M)} < \frac{1}{\left(\frac{\pi k}{\eta}\right)^2 + 1}.$$

3.2. Limiting Behaviour of Domain Length

For this section, we will consider the model system described by (6),(7), and (8) and analyze the behavior as the domain length grows unbounded. Using Corollary 2.4 along with the definition of C'' ,

$$\|C''\|_{L^\infty} = \frac{\beta}{\omega} \max \left[\frac{1+\rho_{\min}^2}{\rho_{\min}(1-\rho_{\min})^2}, \frac{1+\rho_{\max}^2}{\rho_{\max}(1-\rho_{\max})^2} \right]. \quad (70)$$

When a new non-homogeneous solution emerges from the fixed point, $\omega = \omega_k + \epsilon$, we can asymptotically approximate the solutions $\rho = \tilde{M} + \epsilon \rho_1 + O(\epsilon^2) + \epsilon \rho_1 + O(\epsilon^2)$ and $\Phi = \tilde{M} + \epsilon \Phi_1 + O(\epsilon^2) + \epsilon \Phi_1 + O(\epsilon^2)$. Substituting these expansions into (34) and (59), we notice that

$$1 < \frac{\mu_l^2 + 1}{\mu_k^2 + 1} + O(\epsilon) \quad (71)$$

when $l < k$, we get that $l > 1$ implies $\delta \rho = \cos(\mu_l x)$ is an unstable perturbation. So, all non-single step perturbations start out unstable.

Note that an interesting phenomenon happens if we allow the domain length, η , to increase. For a given K , as η approaches infinity, the points $(\Phi_{\min}, 0)$ and $(\Phi_{\max}, 0)$ approach the separatrix at S_1, S_3 , or both. As a result, $\|C''\|_{L^\infty}$ stays bounded for large η .

Looking at (34), we see that as η becomes unbounded every multi-step solution will eventually emerge. Previous phase plane analysis and (60) indicates that if a solution with k -step emerges and is stable in the limit, then all l -step solutions, with $l < k$, will also become stable. In particular the single-step solutions will always stay or become stable if a given k -step solution becomes stable. In practice though, this may require incredibly large values of η .

Also note that $\frac{1+\rho^2}{\rho(1-\rho)^2}$ has a minimum 7.41375 at $\rho = 0.295598$. Thus, if

$$7.41375 > \frac{\omega}{\beta \left(\left(\frac{\pi}{\eta} \right)^2 + 1 \right)},$$

then all stationary solutions are stable by Theorem 3.2. Since Lemma 2.5 is not a strict if and only if statement, we cannot exclude the possible existence of stable non-constant solutions in this region. Furthermore, the constant solution, $(\rho, \Phi) = (M, M)$, is unstable if and only if

$$\frac{1+M^2}{M(1-M)^2} < \frac{\omega}{\beta \left(\left(\frac{\pi}{\eta} \right)^2 + 1 \right)} \text{ using either Theorem 3.2 or condition (60).}$$

3.3. Plateaus vs. Spikes

In this section, we consider the system

$$\rho_\tau = (h(\rho)\rho_s)_s - (g(\rho)v_s)_s \quad (72)$$

$$\Phi_\tau = \Phi_{ss} - \Phi + \rho \quad (73)$$

$$\rho_s(0) = \Phi_s(0) = \rho_s(\eta) = \Phi_s(\eta) = 0. \quad (74)$$

and assume that h and g are chosen such that unique solutions exist and $\rho(\Phi)$ can be well defined as a monotonically increasing function in a similar way as in the case corresponding to (11). As described in [7], the classification of one dimensional local maxima into spikes or plateaus is based on the observations concerning the nonlocal gradient of the first derivative at maxima. In particular, for many qualitative spikes (plateaus) it was observed that the non-local gradient of the first derivative was larger (smaller) than the second derivative.

In this section, we will use the equivalent definition to classify the maximum of stationary solutions of (72, 73) as a spike (plateau) if the fourth derivative of Φ or ρ is positive (negative). For a stationary solution, one can integrate the right hand side of (72) with respect to s , and set the integration constant to zero to satisfy the boundary condition as with (9), to see that critical points of $\rho(s_0) := \rho(s_0, \cdot)$ correspond to critical points $\Phi(s_0) := \Phi(s_0, \cdot)$. Note that if either ρ or Φ is maximum at s_0 , then the assumption that $\rho(\Phi)$ exists, and is monotonically increasing, causes the other to be a maximum, since at a critical point

$$\partial_{ss}\rho(\Phi(s_0)) = \rho'(\Phi(s_0))\partial_{ss}\Phi(s_0).$$

The equilibrium equations yield

$$0 = (h(\rho(s))\rho'(s))' - (g(\rho(s))\Phi'(s))' \quad (75)$$

$$0 = \Phi(s)'' + \rho(s) - \Phi(s). \quad (76)$$

Taking the two derivatives on the top and bottom gives

$$0 = (h\rho')''' - (g(\rho)\Phi')''' \quad (77)$$

$$0 = \Phi^{IV} + \rho'' - \Phi''. \quad (78)$$

Observe that evaluating (75) and (76) at s_0 we get

$$\rho''(s_0) = g\Phi''/h \quad (79)$$

$$\Phi''(s_0) = -\rho + \Phi. \quad (80)$$

Similarly, evaluating (77) and (78) at s_0 allows us to get

$$\rho^{IV}(s_0) = (-3\partial_\rho h(\rho'')^2 + 3\partial_\rho g\rho''\Phi'' + g\Phi^{IV})/h \quad (81)$$

$$\Phi^{IV}(s_0) = -\rho'' + \Phi''. \quad (82)$$

Substituting (79) and (82) into (81), we get

$$\rho^{IV}(s_0) = 3(\Phi'')^2 \frac{g}{h} \frac{(h\partial_\rho g - g\partial_\rho h)}{h^2} + \frac{g}{h} \Phi^{IV} \quad (83)$$

$$= (\Phi'') \frac{g}{h} \left[3\Phi'' \partial_\rho \left(\frac{g}{h} \right) - \frac{g}{h} + 1 \right] \quad (84)$$

since $\Phi''(s_0) < 0$, $g/h > 0$, and by (80) we have $\rho(s_0)$ is a spike if and only if

$$-3(\rho - \Phi) \partial_\rho \left(\frac{g}{h} \right) - \left(\frac{g}{h} - 1 \right) < 0 \quad (85)$$

Recall, $C'' = h/g$ and we can multiply both sides by C'' to rewrite the spike condition as

$$0 < 3(\rho - \Phi) C'' \partial_\rho \left(\frac{1}{C''} \right) + (1 - C'') \quad (86)$$

Notice that $\rho - \Phi > 0$ since we are at maximum. This allows us to write the spike condition for ρ as

$$3 \frac{C'''}{C''} < \left(\frac{1 - C''}{\rho - \Phi} \right) \quad (87)$$

Similarly, the plateau condition is the same inequality, but with the sign reversed.

Now we examine the case when Φ is a plateau. Substituting (79) into (82), we get

$$\Phi^{IV}(s_0) = \left(-\frac{g}{h} + 1 \right) \Phi'' \quad (88)$$

Since $\Phi''(s_0) < 0$, we have $\Phi(s_0)$ is a spike if and only if

$$\frac{g(\rho(s_0))}{h(\rho(s_0))} > 1 \quad (89)$$

For (6) and (7), this is equivalent to

$$\frac{(1 + \rho(s_0)^2)}{\rho(s_0)(1 - \rho(s_0))^2} < \frac{\omega}{\beta}.$$

Also, the plateau condition becomes

$$C'''(\rho(s_0)) > 1.$$

The plateau versus spike condition for Φ looks similar to the condition for stability versus in-stability, except we evaluate at a single point rather than over an integral against a perturbation. Also, we have the right hand side of the plateau condition is larger than the right hand side of the stability condition since

$$1 \geq \|\delta\rho^2\|_{L^2}^2 \quad (90)$$

$$\geq \frac{\eta}{2} \sum_{k>0} A_k^2 \quad (91)$$

$$> \sum_{k>0} A_k^2 \frac{\eta}{2(\mu_k^2+1)} \quad (92)$$

The spike condition

$$C''(\rho(s_0)) < 1,$$

is similar to the condition that the solution becomes unstable as η goes to infinity. In fact, it can be seen that if a periodic solution is a spike, then on a long enough domain it will become unstable. While we cannot state for certain that all unstable solutions are spikes, as some may be plateaus, it is possible to use Theorem 3.2 to see

Corollary 3.3. All non-constant solutions to the system described in (72, 73, 74) that satisfy the instability conditions in Theorem 3.2 have a spike in Φ .

Proof. Use Theorem 3.2 and the fact that the condition on $\|C''\|_{L^\infty}$ is easier to satisfy than the inequality of (89) to get the result.

Notice for our application equation (6), $C'''(\rho) > 0$ is minimum at $\rho^* = 0.295598$. For $\rho(s_0) < \rho^*$, the spike condition for ρ clearly holds when $1 > C''(\rho(s_0))$. Likewise, if $u(s_0)$ is larger than the location of the minimum, e.g., if $M > \rho^*$, the plateau condition holds when $1 < C''(\rho(s_0))$. Otherwise the equation will have to be evaluated to determine if ρ is a plateau or a spike.

Fortunately, in many of the cases that are dealt with numerically, $\rho(s_0) > \rho^*$ and so plateaus for $\Phi(s_0)$ coincide with plateaus for $\rho(s_0)$.

4. Numerics

To demonstrate the existence of stable multi-step solutions as well as analyze the properties of such solutions, we use numerics to evaluate the various expressions as well as solve the PDE. Specifically, we use MATLAB's pdepe code which uses Skeel and Berzin's method for discretizing the spatial domain [16] in order to apply the method of lines coupled with MATLAB's stiff variable order ODE solver, ode15s. For this section, we examine the rescaled system (6–8) for $\omega = 1$ and $\beta = 0.1$.

First, we wish to examine what $C''(\rho)$ looks like. Graphing it, we see a concave up function with two singularities, with the steeper singularity at $\rho = 0$ (see Figure 3a).

If we assume that $S_i = (\Phi, \psi) = (M, 0)$, for $M = 0.25$ and some $i = 1, 2, 3$, then one question

we can ask is, what are the other S_j values, for given K , as we vary $\frac{\beta}{\omega}$. For such fixed points, S_j we have $\psi = 0$, $\Phi_j = \rho_j$, and can use $K = Q(M) - M$ and (11–12) to solve for valid

constant Φ_i . We can then graph the roots of $Q(\Phi) - K - \Phi = 0$ for different values of $\frac{\beta}{\omega}$ (see Figure 3b). For large ratios of diffusion, β , to chemotactic strength, ω , only one constant solution is allowed. As the ratio decreases, we see the emergence of two new steady solutions, and the line for $\Phi = 0.25$ becomes Φ_2 . As the ratio decreases further, the line for $\Phi = 0.25$ switches from being Φ_1 to Φ_2 . This point coincides with the location when

$\frac{\beta}{\omega} \frac{1+M^2}{M(1-M)^2}$ equals 1. Past this point, for sufficiently large domains, $\Phi_2 = M$ becomes unstable.

Note that the different separatrix values are included to give an intuition to the Hamiltonian relationship between solutions with the same K value, not necessarily to indicate a bifurcation in the dynamics as one normally sees in saddle node and transcritical bifurcations. In fact, since the different values of Φ_i correspond to different values of M , it is not possible to dynamically move from one of these constant steady states to another.

Now, we examine solutions to the system. For demonstration purposes, we set the initial conditions of the PDE to be constant, with a small cosine wave perturbation:

$$\rho(s, 0) = 0.25 + 0.05 \cos\left(\frac{\pi}{\eta}s\right),$$

$$\Phi(s, 0) = 0.0125 + 0.0025 \cos\left(\frac{\pi}{\eta}s\right).$$

We allow the function to evolve until time $\tau = 10^{14}$. For small η , the PDE converges to a constant steady state solution. For larger lengths, $\eta = 40$, multi-step structures emerge during a short transition time. These structures display the characteristic meta-stability by remaining almost unchanged for a long period of time. Progressively, these structures transition to smaller and smaller numbers of meta-stable steps until the solution converges to a stable single step. For $\eta = 100$, the end convergence results in a double step pattern (see Figure 4 for single and double step plots). Even though a double step pattern is reached numerically, the solution is not precisely centered. Since periodicity for reflected solutions is preserved, this is still an approximate steady state solution, and most likely happened because the initial conditions were biased to one side of the system. It is interesting that ρ and Φ are almost identical. The differences between them are as small as possible, just to satisfy Eq. (7).

Numerically checking the spike versus plateau conditions for non-stationary solutions $\rho(x, t)$ and $\Phi(x, t)$ at various times indicates that both ρ and Φ satisfy the plateau conditions near the same time for both $\eta = 40$ and $\eta = 100$. Once the solutions satisfy the plateau condition, they continue to satisfy it at later times.

We ran several simulations with varying ω and end time $\tau = 10^{14}$. We then plotted the values of K , $\tilde{M}$, $\sup C''(u(x))$, and $\inf C''(u(x))$ for the resulting steady state solutions (see Figure 5). Changing η between 40 and 100 resulted in little to no qualitative change in these, so the resulting values are plotted for $\eta = 40$. In the first plot, K decreases steadily indicating that the difference between Φ and $Q(\rho)$ is increasing (see Figure 5a). For constant solutions $\tilde{M} = M$, but after the bifurcation that results in $\rho = M$ becoming unstable, the value of $\tilde{M}$ jumps and starts increasing sub-linearly (see Figure 5b). In the final plot, the value $\sup C''$

ρ) increases exponentially while $\inf C''(\rho)$ remains constant since C'' is bounded below and achieves its minimum as ρ changes between peaks and troughs (see Figure 5c). This indicates the above stability conditions in Theorem 3.2 become less useful as β decreases (e.g. if ω increases), and further methods are needed to simplify the more general stability conditions found in (60).

5. Discussion

Under starvation conditions, the chemotactic amoeba, *Dictyostelium discoideum*, is capable of aggregating together and forming slugs. In this paper, we examined a PDE model of the slug formation of the amoeba [11] that does not exhibit blow up in finite time [1, 6]. In particular, we examined what patterns may be generated by the model, when slug formation may occur, and when slug formation versus formation of homogeneous densities would be stable.

We have shown the existence of a Lyapunov function for the PDE model as well as convergence of the solutions of the PDE system to the steady state solutions. The steady state solutions were classified as either constants or bounded sequences of steps. The steps can be plateaus or spikes. A sequence of plateau steps qualitatively resembles the formation of several slugs. Stability conditions are described for both constant and non-constant steady state solutions, as well as for the non-constant, steady state, plateau solutions. Finally, numerical solutions to the PDE system demonstrated transitions in the number of half-steps as either the domain length, or the ratio of chemotactic sensitivity to cell diffusion, increased.

A Hamiltonian characterization of the steady state solutions is also given, but this characterization relies on scalars that are calculated from a given solution, e.g., $\tilde{M}$ and K . Numerically, we see that these scalars vary with the parameters, e.g., the chemical production rate α , or the chemotactic sensitivity χ (entering the reduced system through ω). The dependence of these variables on parameters, such as α and χ , makes it difficult to establish when k -step inhomogeneous solutions exist. Once we have information from one steady state solution, we can use that information, and knowledge about bifurcating periodic orbits, to conjecture the existence of other steady state solutions to the system.

The resulting thresholds, derived from the characterization of the plateau versus spike solutions and unstable versus stable solutions, are close to each other. In the limit, as the domain length approaches infinity, the thresholds approach each other, suggesting that knowledge of whether or not the solution is plateau might determine its stability or visa-versa. However, the condition for stability is global, and requires calculation of an integral over the entire domain, versus the condition for a plateau, which is local. As a result, it is not obvious how to link plateau conditions and stability conditions for an arbitrary inhomogeneous solution. Numerically, the resulting approximate steady state solutions, calculated over long time runs, satisfy both the stability and the plateau conditions, suggesting that stable solutions are plateaus, even if we cannot prove it at this time.

From the biological point of view, it is interesting that, up to normalizing factors, the densities of the cells u and of the chemical v are almost exactly the same. This suggests that not only do cell density and chemical concentrations influence each other, but that they are strongly correlated in how they influence each other at steady states. While future biological experiments will be needed to test this result, we can now hypothesize that cells that maintain consistent chemotactic behavior, when exposed to a constant in time chemotactic pattern, will approximately replicate this pattern.

Based on the results described above, we can predict when a given parameter set will result in constant steady state solutions versus when it will result in formation of patterns, as determined by diffusion of the chemical, its decay and production by the cells, as well as by diffusion of the cells in the chemotactic field. It can be determined whether a given steady state is stable or not, and whether or not it is a plateau. However, there are still many open questions related to this system. In particular, when given only initial conditions, we do not currently know how the resulting variables, K and $\tilde{M}$, can be calculated. Also, additional study is needed to determine how to precisely predict when solutions for a given parameter set, and given k , would approach k -step stable plateaus. This would result in gaining an insight into how environmental parameters influence the number of slugs that form and how wide apart these slugs are.

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6. References

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Figure 1.

With K and $(\rho(\eta), \Phi(\eta))$ calculated from the convergent steady state solution of the PDE, the equation $\Phi = f(\Phi)$ demonstrates (a) one root for $(\rho(\eta), \Phi(\eta)) = (0.25, 0.25)$ and $\omega = 0.7$ or (b) three roots for $(\rho(\eta), \Phi(\eta)) = (0.0499, 0.0499)$ and $\omega = 1$

Figure 2.

Graph of sample Hamiltonian curves using $\omega = 1$, $\beta = 0.1$, $K = -0.1392$, and various $\Phi(0)$ (corresponding to various energy constants H). Trajectories that possibly can and definitely cannot generate stationary solutions to the PDE problem (6), (7), (8) for finite η are colored blue and red respectively.

Figure 3.

a) Graph of $C''(\rho)$ for $\omega = 1$, $\beta = 0.1$ and b) Values of constant solution Φ_i as $\frac{\beta}{\omega}$ increases given one $\Phi_i = M$ for $M = 0.25$

Figure 4. Surface Plots of ρ and Φ over time, in log scale, with a stable single step at $\eta = 40$ and a stable 2-step at $\eta = 100$ with same initial conditions up to scaling in the x -coordinate (a,b,d,e). Density plots for end time values of ρ and Φ at $\tau = 10^{14}$ (c,f)

Figure 5.

Plots of a) K , b) $\tilde{M}$, and c) $\inf C''(\rho)$ and $\sup C''(\rho)$, for the resulting steady state solution, with $\eta = 40$ and varying ω .