# A MODEL BIOCHEMICAL REACTION

Thesis by

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## Abstract

Asymptotic solutions are presented to the non-linear parabolic reaction-diffusion equations describing a model biochemical reaction proposed by I. Prigogine. There is a uniform steady state which, for certain values of the adjustable parameters, may be unstable. When the uniform solution is slightly unstable, the two-timing method is used to find the bifurcation of new solutions of small amplitude. These may be either non-uniform steady states or time-periodic solutions, depending on the ratio of the diffusion coefficients. In the limit that one of the diffusion coefficients is infinite, multiple steady states of finite amplitude are found. When one of the parameters is allowed to depend on space and the basic state is unstable, it is found that the non-uniform steady state which is approached may show localized spatial oscillations. The localization arises out of the presence of turning points in the linearized stability equations. When diffusion is absent it is shown how kinematic concentration waves arise. Detailed calculations using singular perturbation techniques are made of the basic oscillation giving rise to these waves, which is a relaxation oscillation. It is found that the equations in its asymptotic approximation are not obtained from the full equations as the result of a limit process.

# Contents

## 0.1. Introductory Remarks

Under certain circumstances, the usual equilibrium state of a chemical reaction may be unstable with respect to small changes in the concentrations, or to other perturbations. There is a variety of phenomena which may occur in the subsequent development of the reaction. Experimental work has shown that these include self-sustaining oscillations in concentration; concentration waves; and the establishment of new steady states which are not uniform. Aside from their intrinsic interest, these phenomena have implications in the study of circadian rhythms, morphogenesis, and pre-biological evolution. However, their prediction and quantitative description clearly require a detailed knowledge of the reaction mechanism; this is in most cases lacking. Accordingly, we study a model biochemical reaction, with known kinetics, which is described ultimately by the pair of coupled parabolic equations

$$\frac{\partial X}{\partial t} = A - (B+1)X + X^2Y + D_X \frac{\partial^2 X}{\partial r^2} ,$$

$$\frac{\partial Y}{\partial t} = BX - X^2Y + D_Y \frac{\partial^2 Y}{\partial r^2} .$$

The model is due to I. Prigogine. Numerical studies have shown that, depending on the parameters A, B, $D_X$ and $D_Y$, the equations can exhibit both concentration waves and non-uniform steady states. A remarkable feature is that when the parameter A (which represents the concentration of another reactant) is allowed to depend on the space variable r, the region of instability is localized in space.

The present work uses perturbation techniques to calculate asymptotic solutions to the rate equations and show how these phenomena can occur. In the next section we describe the model more precisely, define the governing equations, and summarize the numerical results of Herschkowitz-Kaufman and Nicolis [3].

## 0.2. Detailed Description of the Model

The model reaction introduced by Prigogine is $A+B \rightarrow D+E$ according to the sequence

$$A \rightarrow X$$
$$2X + Y \rightarrow 3X$$
$$B + X \rightarrow Y + D$$
$$X \rightarrow E \ .$$

It is thought not to represent any known biochemical reaction, but, as mentioned above, does exhibit some of their important features. The simplest possible assumption is made about the rate of reaction: namely, that it is proportional to the correct product of the concentrations. Thus the presence of the autocatalytic step $2X+Y \rightarrow 3X$ makes the rate equations non-linear, since the rate of production of reactant X from this step is proportional to $[X]^2[Y]$. A further simplifying assumption is made by setting all the rate constants equal to one. This means in particular that temperature variations have been completely neglected; such an assumption seems not unreasonable, since chemical reactions going on in living tissue cannot be very exothermic. Also, it is supposed that there is no convective motion of the reactants, and back reactions are neglected. Then the conservation equations for the concentrations A, B, X, Y, D, E are

$$\frac{\partial A}{\partial t} = -A + D_A \nabla^2 A$$

$$\frac{\partial B}{\partial t} = -BX + D_B \nabla^2 B$$

$$\frac{\partial X}{\partial t} = A + X^2Y - BX - X + D_X \nabla^2 X$$

$$\frac{\partial Y}{\partial t} = -X^2Y + BX + D_Y \nabla^2 Y$$

$$\frac{\partial D}{\partial t} = BX + D_D \nabla^2 D$$

$$\frac{\partial E}{\partial t} = X + D_E \nabla^2 E \ .$$

We have written X instead of [X] for the concentration of reactant X, and so forth, since there can be no risk of ambiguity. The D's are diffusion coefficients. It will be noticed that the equation for A is not coupled to the rest so that it may be solved first. Further, the equations for D and E become merely inhomogeneous linear equations once those for B, X, and Y have been solved. Actually Herschkowitz-Kaufman and Nicolis [3] make the further assumption that the concentration of B is somehow maintained uniform (alternatively, $D_B = \infty$) so that B appears only parametrically in the equations for X and Y. Also, they take $D_A$ to be fairly large so that A relaxes fairly quickly to its steady state. They then substitute this steady state value of A into the equation for X, and consider the reaction to be taking place in an infinite slab of width 1. The differential equations which they consider are thus

$$\frac{\partial X}{\partial t} = A(r) - (B+1)X + X^2Y + D_X \frac{\partial^2 X}{\partial r^2} \qquad (0.2.1)$$

$$\frac{\partial Y}{\partial t} = BX - X^2Y + D_Y \frac{\partial^2 Y}{\partial r^2} \ , \qquad (0.2.2)$$

where r is the spatial co-ordinate and

$$A(r) = \overline{A}\ \mathrm{sech}\ \frac{1}{\sqrt{D_A}}\ \cosh\ \frac{r-\frac{1}{2}}{\sqrt{D_A}}\ .$$

They pick $D_A = 197 \times 10^{-3}$, $D_X = 1.05 \times 10^{-3}$, $\overline{A} = 14$ and allow B and $D_Y$ to be free parameters. The boundary conditions are that $X(0,t) = X(1,t) = \overline{A}$ and $Y(0,t) = Y(1,t) = B/\overline{A}$.

In the limit $D_A = \infty$, so that $A(r) \equiv \text{const.} = \overline{A}$, there is a uniform steady state $X(r,t) \equiv \overline{A}$, $Y(r,t) \equiv B/\overline{A}$. When A(r) is not constant, and $D_X$ and $D_Y$ are small, there is a steady state $X \sim A(r) + O(D_X, D_Y)$, $Y \sim B/A(r) + O(D_X, D_Y)$. This might be called the basic steady state. (See figure 0.2.1.) It should be noticed that the boundary conditions have been chosen in such a manner that the basic state satisfies them. Thus no boundary layers occur at the edges of the slab, even though $D_X$ and $D_Y$ are small and multiply the highest-order derivatives. Herschkowitz-Kaufman and Nicolis find that for certain values of the parameters B and $D_Y$ the basic state is unstable against small perturbations in the initial conditions. The subsequent development of the system can lead either to a new steady state which shows spatial oscillations ("dissipative structure") or to propagating waves of concentration. Figure 0.2.2 shows the dissipative structure that is found for the choices $D_Y = 5.25 \times 10^{-3}$, $B = 26$. Figures 0.2.3 through 0.2.6 show several concentration profiles in the course of one oscillation in the time-periodic solution that is found for the choices $D_Y = .66 \times 10^{-3}$, $B = 77$. These pictures have been copied from the

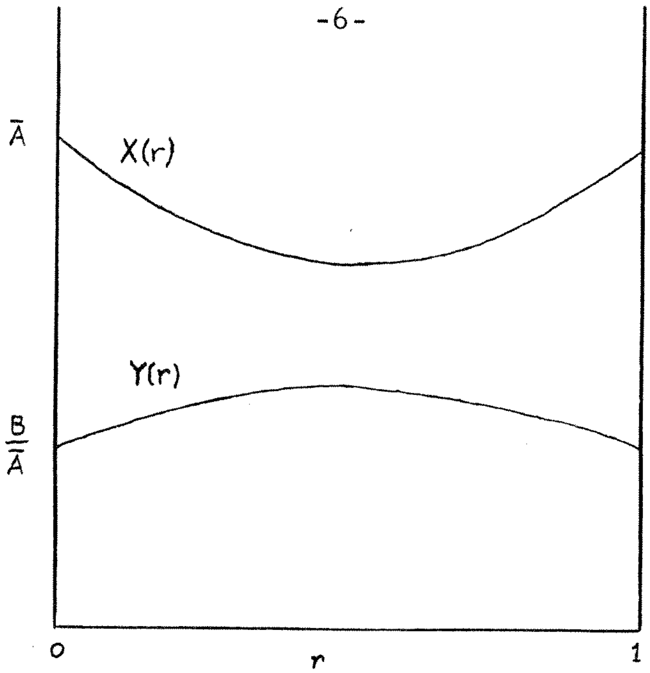


Figure 0.2.1. The basic steady state.

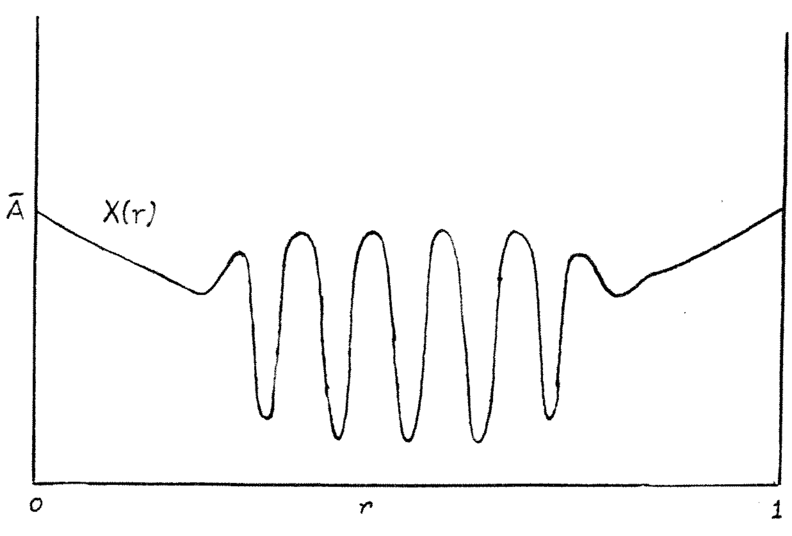


Figure 0.2.2. A localized dissipative structure.

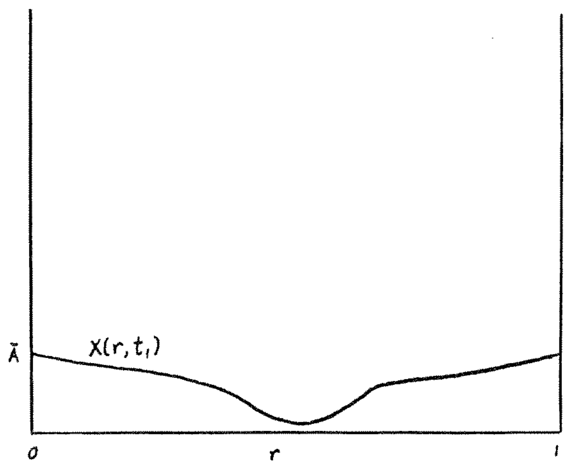


Figure 0. 2. 3

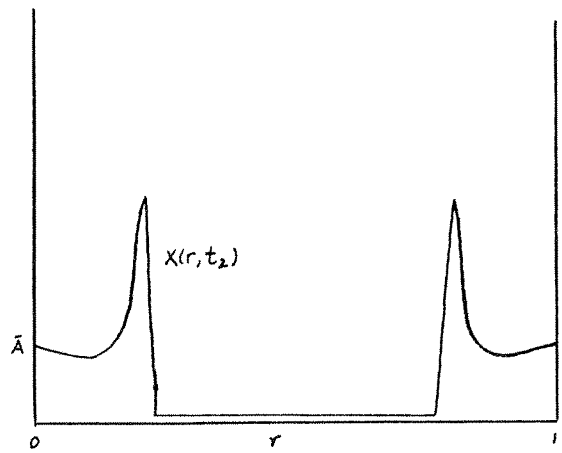


Figure 0. 2. 4

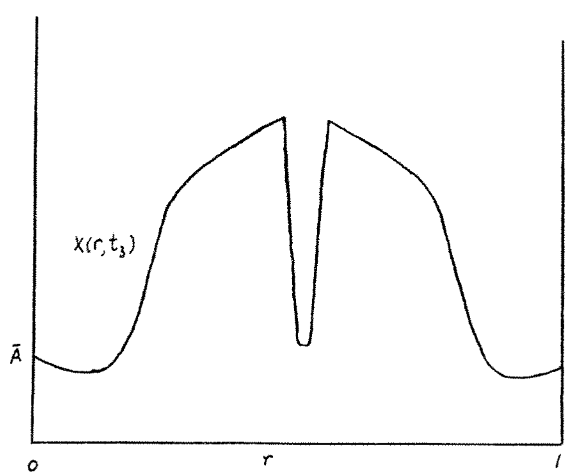


Figure 0. 2. 5

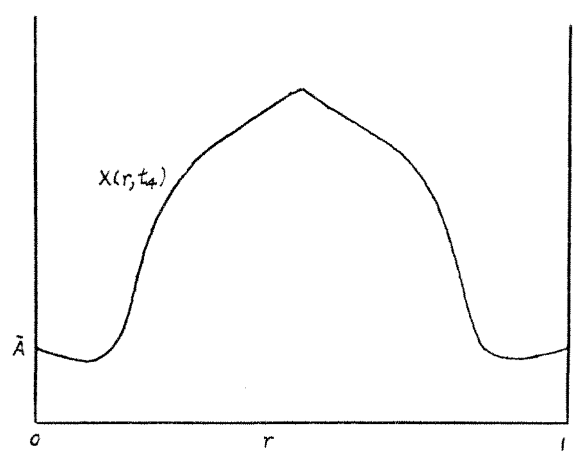


Figure 0. 2. 6

Several concentration profiles in the course of one oscillation.

paper of Herschkowitz-Kaufman and Nicolis. In each case the disturbance from the basic state is confined to the centre of the slab so that the instability of the basic state can be considered local. This localization is clearly due to the non-uniform distribution of reactant A.

In attempting to explain the localization we shall take advantage of the fact that $D_X << 1$ and $D_Y << 1$. The natural length scale on which X may be expected to vary appreciably is $D_X^{\frac{1}{2}}$, whereas A varies on a length scale of $D_A^{\frac{1}{2}}$. The ratio of these quantities is

$$(D_X/D_A)^{\frac{1}{2}} = (1.05 \times 10^{-3}/197 \times 10^{-3})^{\frac{1}{2}} \approx 1/14 ,$$

so that variations in A can be considered slow compared to those in X. The case in which A is uniformly distributed is also of interest, since solutions can exhibit both non-uniform steady states and waves, although not localization.

Accordingly, the plan of this thesis is as follows. Chapter 1 considers the case of constant A and shows how waves and dissipative structures may occur. In Chapter 2 we allow A to be non-constant and attack the problem of localization. Chapter 3 offers some opinions about the biological significance of the model.

## 1. Non-Localized Disturbances

Throughout this chapter the concentration of reactant A is taken to be constant and equal to $\overline{A}$.

### 1.1 Stability of the Uniform State

When A is constant, equations (0.2.1) and (0.2.2) become

$$\frac{\partial X}{\partial t} = A - (B+1)X + X^2Y + D\frac{\partial^2 X}{\partial r^2}, \qquad (1.1.1)$$

$$\frac{\partial Y}{\partial t} = BX - X^2Y + \vartheta D\frac{\partial^2 Y}{\partial r^2}, \qquad (1.1.2)$$

and the boundary conditions are $X(0,t) = X(1,t) = A$, $Y(0,t) = Y(1,t) = B/A$. Here we have written D for $D_X$ and $\vartheta$ for $D_Y/D_X$. It is seen that (1.1.1) and (1.1.2) possess a unique uniform solution $X \equiv A$, $Y \equiv B/A$, which satisfies the boundary conditions. The linearized stability of this solution can be found by standard methods. If we write $X = A+u$, $Y = B/A + v$, and omit terms quadratic or higher in u and v, the linearized differential equations for u and v are

$$\frac{\partial u}{\partial t} = (B-1)u + A^2v + D\frac{\partial^2 u}{\partial r^2}, \qquad (1.1.3)$$

$$\frac{\partial v}{\partial t} = -Bu - A^2v + \vartheta D\frac{\partial^2 v}{\partial r^2}, \qquad (1.1.4)$$

together with the boundary conditions $u(0,t) = u(1,t) = v(0,t) = v(1,t) = 0$. We look for solutions of the form $u(r,t) = e^{\sigma t}\phi(r)$, $v(r,t) = e^{\sigma t}\psi(r)$. The equations for $\phi$ and $\psi$ are thus

$$\sigma\phi = (B-1)\phi + A^2\psi + D\phi'', \qquad (1.1.5)$$

$$\sigma\psi = -B\phi - A^2\psi + \vartheta D\psi'', \qquad (1.1.6)$$

with boundary conditions $\phi(0) = \phi(1) = \psi(0) = \psi(1) = 0$. This eigenvalue problem will have a solution only for certain values of $\sigma$. If the vector eigenfunction associated with the eigenvalue $\sigma_n$ is $[\phi_n, \psi_n]^t$, then the solution of (1.1.3) and (1.1.4) will be

$$\begin{bmatrix} u \\ \\ v \end{bmatrix} = \mathrm{Re} \sum_{n=1}^{\infty} c_n e^{\sigma_n t} \begin{bmatrix} \phi_n(r) \\ \\ \psi_n(r) \end{bmatrix} ,$$

when the coefficients $c_n$ are determined from the initial conditions. The uniform state is then called stable if Re $\sigma_n < 0$ for all n; unstable if Re $\sigma_m > 0$ for some m; and "neutrally stable" if Re $\sigma_m = 0$ for one value of m, but all other $\sigma_n$ have Re $\sigma_n < 0$.

Since (1.1.5) and (1.1.6) have constant coefficients, we try solutions in sines. First we rewrite the equations in the form

$$\begin{bmatrix} D\phi'' \\ \\ \vartheta D\psi'' \end{bmatrix} = \begin{bmatrix} \sigma-(B-1) & -A^2 \\ \\ B & \sigma+A^2 \end{bmatrix} \begin{bmatrix} \phi \\ \\ \psi \end{bmatrix} , \qquad (1.1.7)$$

and then try $\phi = \sin n\pi r$, $\psi = M_n \sin n\pi r$, so that $\phi'' = -n^2\pi^2\phi$ and $\psi'' = -n^2\pi^2\psi$. Equation (1.1.7) becomes

$$\begin{bmatrix} -n^2\pi^2 D\phi \\ \\ -n^2\pi^2 \vartheta D\psi \end{bmatrix} = \begin{bmatrix} \sigma-(B-1) & -A^2 \\ \\ B & \sigma+A^2 \end{bmatrix} \begin{bmatrix} \phi \\ \\ \psi \end{bmatrix},$$

or

$$\begin{bmatrix} \sigma-(B-1)+n^2\pi^2 D & -A^2 \\ B & \sigma+A^2+n^2\pi^2 \vartheta D \end{bmatrix} \begin{bmatrix} \phi \\ \psi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} . \qquad (1.1.8)$$

There will be non-trivial solutions to (1.1.8) only if the determinant of the coefficients is zero; that is, if

$$[\sigma-(B-1) + n^2\pi^2 D]\ [\sigma+A^2+n^2\pi^2\vartheta D] + A^2 B = 0 ,$$

or

$$\sigma^2+\sigma[-B+1+A^2+n^2\pi^2 D(1+\vartheta)]$$
$$+ A^2B+[A^2+n^2\pi^2\vartheta D]\ [-(B-1)+n^2\pi^2 D] = 0 . \qquad (1.1.9)$$

Let us now change the notation slightly. Associated with each value of n there will be two eigenvalues which are the roots of (1.1.9). They may be real or complex conjugate, depending on the parameters $\vartheta$ and B. We call them $\sigma_n^+$ and $\sigma_n^-$, according to the definition

$$\sigma_n^{\pm} = \frac{1}{2}\left\{B-1-A^2-n^2\pi^2 D(1+\vartheta) \pm \left[[B-1+A^2+n^2\pi^2 D(\vartheta-1)]^2-4A^2B\right]^{\frac{1}{2}}\right\} . \qquad (1.1.10)$$

The eigenfunction corresponding to $\sigma_n^{\pm}$ will be called $\underline{\phi}_n^{\pm} = [\phi_n^{\pm},\psi_n^{\pm}]^t$. The functions $\psi_n^{\pm}$ will be given by $\psi_n^{\pm} = M_n^{\pm} \sin n\pi r$, where from (1.1.8)

$$\sigma_n^{\pm} - (B-1) + n^2\pi^2 D - A^2 M_n^{\pm} = 0 .$$

While it is clear that the real part of $\sigma_n^+$ is always greater than or equal to the real part of $\sigma_n^-$ (with equality if they are complex), it turns out that $\sigma_1^+$ is not necessarily the eigenvalue with the greatest real part. We now show this.

First consider the case $\vartheta = 0$. Then (1.1.10) gives

$$\sigma_n^+ = \frac{1}{2}\{B-1-A^2-n^2\pi^2D+[(B-1-A^2-n^2\pi^2D)^2-4A^2B]^{\frac{1}{2}}\} .$$

The point of neutral stability for $\sigma_n^+$ at $\vartheta = 0$ is at $B = 1+A^2+n^2\pi^2D$. The argument of the surd is then negative so that $\sigma_n^+$ is complex as its real part changes sign. By continuity it follows that the curve of neutral stability for $\sigma_n^+$ in the $\vartheta$, B plane will, for sufficiently small values of $\vartheta$ (which will depend on n), be that which is obtained when $\sigma_n^+$ is complex. That is to say, the curve of neutral stability for $\sigma_n^+$ for small $\vartheta$ is

$$\text{Re}\,\sigma_n^+ = \tfrac{1}{2}[B-1-A^2-n^2\pi^2D(1+\vartheta)] = 0 ,$$

i.e.

$$B = 1 + A^2 + n^2\pi^2D(1+\vartheta) . \qquad (1.1.11)$$

This is a straight line in the $\vartheta$, B plane with slope $n^2\pi^2D$ and B-intercept $1+A^2+n^2\pi^2D$. It will also be the neutral stability curve for $\sigma_n^-$ for complex values of $\sigma_n^\pm$. These lines are shown in figure 1.1.1. The line corresponding to $n = 1$ is the lowest of these, and so for small $\vartheta$, $\sigma_1^\pm$ are the eigenvalues with the greatest real part ("leading eigenvalues") and the curve of neutral stability for the uniform solution is

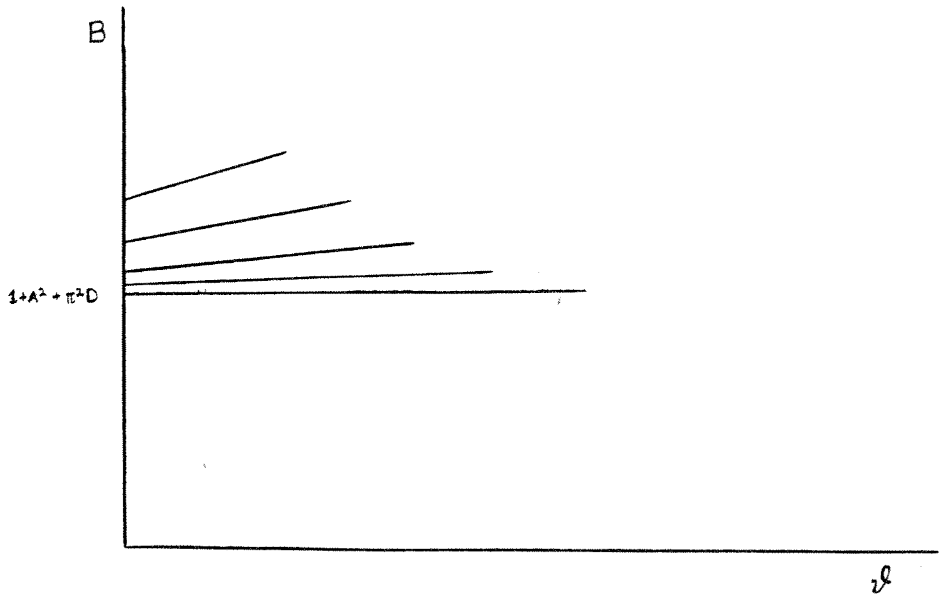


Figure 1.1.1. Neutral stability curves for complex eigenvalues.

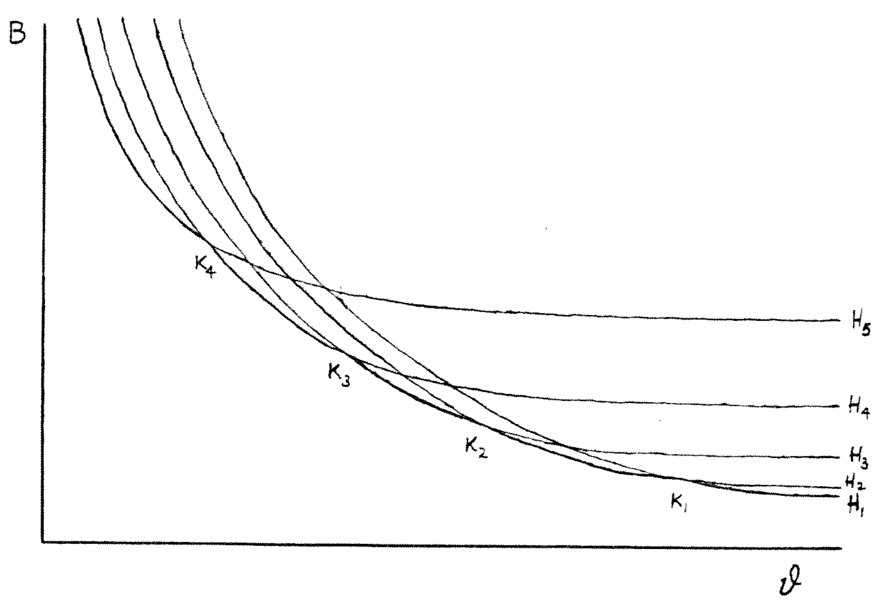


Figure 1.1.2. Neutral stability curves for real eigenvalues.

$$B = 1+A^2+\pi^2 D(1+\vartheta) \quad . \tag{1.1.12}$$

This line will continue to be the neutral stability curve until it intersects one of the neutral stability curves which are obtained for real values of eigenvalues $\sigma_n^{\pm}$.

If $\sigma_n^+$ is real, then the curve of neutral stability for $\sigma_n^+$ in the $\vartheta$, B plane is given by $\sigma_n^+ = 0$, i.e.

$$B = 1+n^2\pi^2 D + \frac{A^2}{\vartheta}\left\{1 + \frac{1}{n^2\pi^2 D}\right\} \quad . \tag{1.1.13}$$

For each n this is a rectangular hyperbola which we shall call $H_n$. As $\vartheta$ tends to infinity, $H_n$ asymptotes to the horizontal line $B = 1+n^2\pi^2 D$. Thus for sufficiently large $\vartheta$, $H_{n+1}$ lies above $H_n$ for every n. However, as $\vartheta$ tends to zero each $H_n$ asymptotes to the B-axis. For each n it is possible to find a value $\vartheta = \vartheta_o(n)$ sufficiently small that $H_n$ lies above $H_{n+1}$ for all $\vartheta < \vartheta_o(n)$. Thus every hyperbola $H_n$ must intersect all the others; the $H_n$ are shown in figure 1.1.2. The neutral stability curve R for the uniform solution that is obtained when the leading eigenvalue is real, is thus given by those portions of hyperbolas $H_n$ which lie the lowest in the $\vartheta$, B plane for given values of $\vartheta$; it is scallop-shaped. It is seen from figure 1.1.2 that every hyperbola $H_n$ has some portion of it on R.

The places where R is not smooth are the points $K_n$ where $H_n$ and $H_{n+1}$ intersect. They are given from (1.1.3) by

$$n^2\pi^2 D + \frac{A^2}{\vartheta}\left\{1 + \frac{1}{n^2\pi^2 D}\right\} = (n+1)^2\pi^2 D + \frac{A^2}{\vartheta}\left\{1+ \frac{1}{(n+1)^2\pi^2 D}\right\} ,$$

or

$$\vartheta = \frac{A^2}{n^2(n+1)^2(\pi^2 D)^2} \quad . \tag{1.1.14}$$

The value of B at $K_n$ is therefore

$$B = 1 + n^2\pi^2 D + (n+1)^2\pi^2 D + n^2(n+1)^2(\pi^2 D)^2 \; .$$

The neutral stability curve for the uniform solution will be given by (1.1.12) until that curve intersects R; then R will replace it, since it then lies below the straight line (1.1.12). The point of intersection will depend on the values of A and D. For $A = 8.22$ (which is the minimum value of A(r) chosen by Herschkowitz-Kaufman and Nicolis [3] ) and $D = 1.05 \times 10^{-3}$, we find that $K_{26}$ lies below (1.1.12) for $0 \leq \vartheta \leq 10$, while $K_{27}$ lies above it. Thus in this case, the neutral stability curve contains portions of hyperbolas $H_1$ through $H_{27}$, but not of $H_n$ for $n > 27$. The point of intersection of (1.1.12) with R is therefore given by the solution of equations (1.1.12), and (1.1.13) with $n = 27$. Using the above values of A and D we find $\vartheta = 1.274$; this is similar to the value of $\vartheta$ found numerically by Herschkowitz-Kaufman and Platten [4] in the case that A varies with r.

Figure 1.1.3 shows the stability regions of the uniform solution in the $\vartheta$, B plane. In region I, below the neutral stability curve, the uniform solution is stable. In region II the uniform solution is unstable, but none of the positive eigenvalues has a non-zero imaginary part. (The upper boundary of region II is the neutral stability curve for $\sigma_1^+$.) In region III the uniform solution is unstable and eigenvalues with positive real part may have a non-zero imaginary

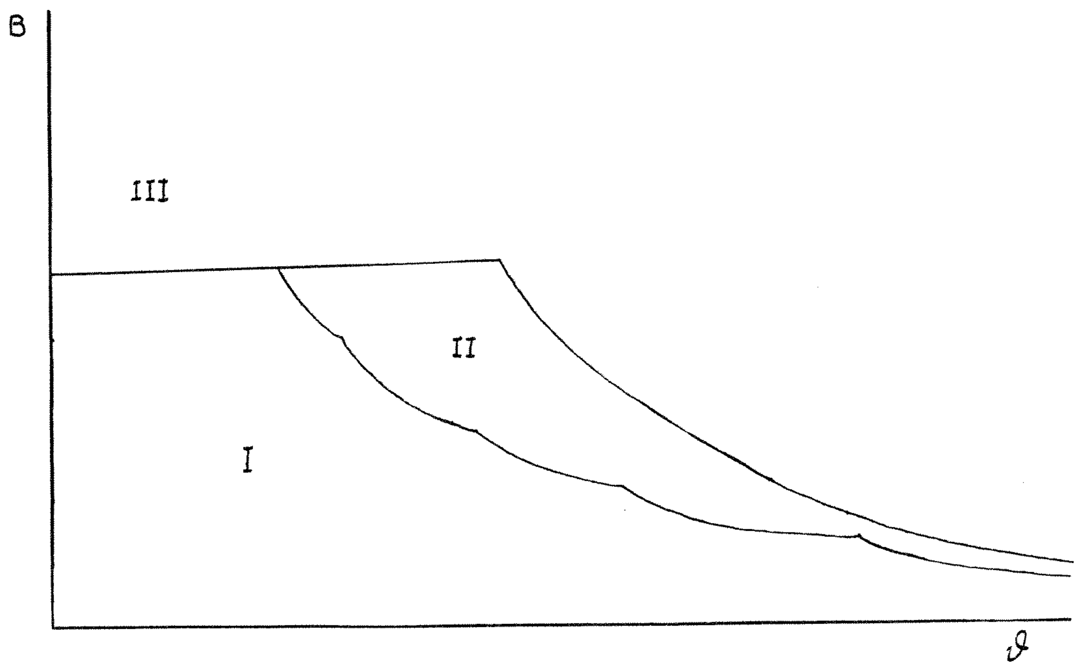


Figure 1. 1. 3. Stability regions of the uniform solution.

part. This is certainly true immediately above the line given by (1.1.12).

In the next sections we shall examine solutions of (1.1.1) and (1.1.2) in several cases when the uniform state is unstable. In section 1.2 we look at the case when the point $\mathcal{D}$, B is only slightly above the neutral stability curve in region II of figure 1.1.3, and consider the bifurcation of non-uniform steady states. In section 1.3 we take $\mathcal{D} \gg 1$ and show how many non-uniform steady states can exist. In section 1.4 we consider the bifurcation of periodic solutions when the point $\mathcal{D}$, B is slightly above the neutral stability curve in region III of figure 1.1.3. Finally in section 1.5 we show how concentration waves can exist if diffusion is absent.

## 1.2. Bifurcation of Non-uniform Steady States

For convenience we rewrite equations (1.1.1) and (1.1.2):

$$\frac{\partial X}{\partial t} = A-(B+1)\,X + X^2Y + D\,\frac{\partial^2 X}{\partial r^2}\ , \tag{1.1.1}$$

$$\frac{\partial Y}{\partial t} = BX - X^2Y + \mathcal{S}D\,\frac{\partial^2 Y}{\partial r^2}\ ; \tag{1.1.2}$$

the boundary conditions are $X(0,t) = X(1,t) = A$ and $Y(0,t) = Y(1,t) = B/A$. In this section we use the two-timing method to study the time evolution of solutions to (1.1.1) and (1.1.2) when the uniform state is unstable and the point $\mathcal{S}, B$ is only slightly above the neutral stability curve in the $\mathcal{S}, B$ plane and in region II of figure 1.1.3. The method was first used in this connection by Matkowsky [ 9 ] and was elaborated on by Kogelman and Keller [5]. We follow Kogelman and Keller's analysis. It will be shown that solutions tend to a new, non-uniform steady state of small amplitude. The amplitude is related (not necessarily linearly) to the small quantity $B-B_c$, where $B_c$ is the value of B on the neutral stability curve. The parameter $\mathcal{S}$ is held fixed in this procedure. The form of the new steady state depends on $\mathcal{S}$. If $\mathcal{S}, B_c$ is not one of the points $K_N$ where the hyperbolas $H_N$ and $H_{N+1}$ intersect, then to first order the new steady state is a multiple of the eigenfunction $\underline{\phi}_N^+$, where N takes on the proper value. If $\mathcal{S}, B_c$ is one of the points $K_N$, then the new steady state is (sometimes) a linear combination of the eigenfunctions $\underline{\phi}_N^+$ and $\underline{\phi}_{N+1}^+$. The analysis when the point $\mathcal{S}, B$ is slightly above the neutral stability curve but in region III of figure 1.1.3 is slightly different, and we do that in section 1.4.

We suppose that initial conditions are given of the form

$$X(r, 0) = A + h(r, \varepsilon) ,$$

$$Y(r, 0) = \frac{B}{A} + k(r, \varepsilon) ,$$

where $h(r, \varepsilon)$ and $k(r, \varepsilon)$ are functions which satisfy $h(r, 0) = k(r, 0) = 0$, $h(0, \varepsilon) = h(1, \varepsilon) = k(0, \varepsilon) = k(1, \varepsilon) = 0$, and $\varepsilon$ is a small parameter. We seek solutions which deviate from the uniform solution by $O(\varepsilon)$ when B exceeds the critical value $B_c = B_c(A, D, \vartheta)$ given by (1.1.13). The amount by which B is greater than $B_c$ will depend somehow (not necessarily linearly) on $\varepsilon$. Alternatively, we could suppose that B exceeds $B_c$ by an amount $\delta$ and then seek solutions deviating from the uniform solution by some small amount which is a function (not necessarily a linear function) of $\delta$. The two views are equivalent.

The two times to be used in the perturbation calculation are the fast time $t^* = t$ and the slow time $\tau = (B(\varepsilon) - B_c)t$. The solutions to (1.1.1) and (1.1.2) are to be given by the asymptotic expansions

$$X \sim A + \varepsilon u_1(r, t, \tau) + \varepsilon^2 u_2(r, t, \tau) + \ldots , \tag{1.2.1}$$

$$Y \sim \frac{B}{A} + \varepsilon v_1(r, t, \tau) + \varepsilon^2 v_2(r, t, \tau) + \ldots , \tag{1.2.2}$$

with the boundary conditions $u_j(0, t, \tau) = u_j(1, t, \tau) = v_j(0, t, \tau) = v_j(1, t, \tau) = 0$ and the initial conditions

$$u_j(r, 0, 0) = \frac{1}{j!} \frac{\partial^j h(r, 0)}{\partial \varepsilon^j} ,$$

$$v_j(r, 0, 0) = \frac{1}{j!} \frac{\partial^j k(r, 0)}{\partial \varepsilon^j} .$$

Substitution of the expansions (1.2.1) and (1.2.2) into equations (1.1.1) and (1.1.2) yields the following hierarchy of equations:

$$\frac{\partial u_1}{\partial t} = (B_c - 1)\, u_1 + A^2 v_1 + D \frac{\partial^2 u_1}{\partial r^2} , \tag{1.2.3}$$

$$\frac{\partial v_1}{\partial t} = -B_c u_1 - A^2 v_1 + \vartheta D \frac{\partial^2 v_1}{\partial r^2} ; \tag{1.2.4}$$

$$\frac{\partial u_2}{\partial t} = (B_c - 1) u_2 + A^2 v_2 + D \frac{\partial^2 u_2}{\partial r^2} - B'(0) \frac{\partial u_1}{\partial \tau} + B'(0) u_1 + \frac{B_c}{A} u_1^2 + 2 A u_1 v_1 , \tag{1.2.5}$$

$$\frac{\partial v_2}{\partial t} = -B_c u_2 - A^2 v_2 + \vartheta D \frac{\partial^2 v_2}{\partial r^2} - B'(0) \frac{\partial v_1}{\partial \tau} - B'(0) u_1 - \frac{B_c}{A} u_1^2 - 2 A u_1 v_1 ; \tag{1.2.6}$$

$$\frac{\partial u_3}{\partial \tau} = (B_c - 1) u_3 + A^2 v_3 + D \frac{\partial^2 u_3}{\partial r^2} - B'(0) \frac{\partial u_2}{\partial \tau} - \frac{B''(0)}{2} \frac{\partial u_1}{\partial \tau} + \frac{B''(0)}{2} u_1 + B'(0) u_2 + \frac{B'(0)}{A} u_1^2 + u_1^2 v_1 + 2 A u_1 v_2 + 2 A u_2 v_1 + \frac{2 B_c}{A} u_1 u_2 , \tag{1.2.7}$$

$$\frac{\partial v_3}{\partial t} = -B_c u_3 - A^2 v_3 + \vartheta D \frac{\partial^2 v_3}{\partial r^2} - B'(0) \frac{\partial v_2}{\partial \tau} - \frac{B''(0)}{2} \frac{\partial v_1}{\partial \tau} - \frac{B''(0)}{2} u_1 - B'(0) u_2 - \frac{B'(0)}{A} u_1^2 - u_1^2 v_1 - 2 A u_1 v_2 - 2 A u_2 v_1 - \frac{2 B_c}{A} u_1 u_2 . \tag{1.2.8}$$

The solution of (1.2.3) and (1.2.4) is then given by the series

$$\begin{bmatrix} u_1 \\ \\ v_1 \end{bmatrix} = \mathrm{Re} \sum_{n=1}^{\infty} \left\{ c_n^+(\tau) \exp(\sigma_n^+ t) \begin{bmatrix} \phi_n^+ \\ \\ \psi_n^+ \end{bmatrix} + c_n^-(\tau) \exp(\sigma_n^- t) \begin{bmatrix} \phi_n^- \\ \\ \psi_n^- \end{bmatrix} \right\} , \tag{1.2.9}$$

where $\sigma_n^{\pm}$ and $[\phi_n^{\pm}, \psi_n^{\pm}]^t$ are the eigenvalues and eigenfunctions found in section 1.1. The initial values of the coefficients $c_n^{\pm}(\tau)$ are found from the initial conditions in the following manner. Let $\hat{\underline{\phi}}_n^{\pm} = [\hat{\phi}_n^{\pm}, \hat{\psi}_n^{\pm}]^t$ be the eigenfunctions of the differential equations adjoint to (1.1.5) and (1.1.6), corresponding to the eigenvalues $\overline{\sigma_n^{\pm}}$. It is easily seen that they are of the form $\hat{\phi}_n^{\pm} = \sin n\pi r$, $\hat{\psi}_n^{\pm} = N_n^{\pm} \sin n\pi r$, where

$$\overline{\sigma_n^{\pm}} - (B-1) + n^2\pi^2 D + BN_n^{\pm} = 0 \; .$$

Thus

$$N_n^{\pm} = -\frac{A^2}{B} \overline{M_n^{\pm}} \; .$$

The inner product of the eigenvectors $\underline{\phi}_n^{\pm}$ and $\hat{\underline{\phi}}_m^{\pm}$ will be given by

$$\begin{aligned} \langle \hat{\underline{\phi}}_m^{\pm} | \underline{\phi}_n^{\pm} \rangle &= \int_0^1 (\overline{\hat{\phi}_n^{\pm}} \, \phi_m^{\pm} + \overline{\hat{\psi}_n^{\pm}} \, \psi_m^{\pm}) \, dr \\ &= \int_0^1 (\sin n\pi r \sin m\pi r - \frac{A^2}{B} M_n^{\pm} M_m^{\pm} \sin n\pi r \sin m\pi r) dr \\ &= \tfrac{1}{2} (1 - \frac{A^2}{B} M_n^{\pm} M_m^{\pm}) \delta_{mn} \; . \end{aligned}$$

It can be shown from (1.1.10) and the definition of $M_n^{\pm}$ that $M_n^+ M_n^- = \frac{B}{A^2}$. Thus distinct eigenfunctions are orthogonal, and an arbitrary function $\underline{f}$ has the expansion

$$\underline{f} = \sum_{n=1}^{\infty} (a_n^+ \underline{\phi}_n^+ + a_n^- \underline{\phi}_n^-) ,$$

where the coefficients are given by

$$a_n^{\pm} = \frac{2\langle \hat{\underline{\phi}}_n^{\pm} \mid \underline{f} \rangle}{1 - \frac{A^2}{B}(M_n^{\pm})^2} .$$

In particular, we obtain

$$c_n^+(0) = \frac{2\int_0^1 \left\{h_\varepsilon(r,0) - \frac{A^2}{B_c} M_n^+ k_\varepsilon(r,0)\right\} \sin n\pi r \, dr}{1 - \frac{A^2}{B_c}(M_n^+)^2} \tag{1.2.10}$$

and

$$c_n^-(0) = \frac{2\int_0^1 \left\{h_\varepsilon(r,0) - \frac{A^2}{B_c} M_n^- k_\varepsilon(r,0)\right\} \sin n\pi r \, dr}{1 - \frac{A^2}{B_c}(M_n^-)^2} \tag{1.2.11}$$

First consider the usual case, when $\mathcal{S}, B_c$ is not one of the points $K_N$. The neutral stability curve will then be a portion of the hyperbola $H_N$ for the relevant value of N. The eigenvalue with the greatest real part when $B = B_c$ will be $\sigma_N^+$; it will be equal to zero, and all other eigenvalues will have negative real parts. Consequently, all terms in the sum in the expansion (1.2.9), except the one corresponding to $\sigma_N^+$, are exponentially decreasing in the fast time t. Thus any variations in the coefficients $c_n^{\pm}(\tau)$ (except $c_N^{+}(\tau)$) are unimportant, and we may without loss of generality set them identically equal to their initial values. The expansion (1.2.9) then becomes

$$\begin{bmatrix} u_1 \\ \\ v_1 \end{bmatrix} = c_N^{+}(\tau)\begin{bmatrix} \sin N\pi r \\ \\ M_N^{+}\sin N\pi r \end{bmatrix} + c_N^{-}(0)\exp(\sigma_N^{-}t)\begin{bmatrix} \phi_N^{-} \\ \\ \psi_N^{-} \end{bmatrix} + \mathrm{Re}\sum_{n\neq N} c_n^{\pm}(0)\exp(\sigma_n^{\pm}t)\begin{bmatrix} \phi_n^{\pm} \\ \\ \psi_n^{\pm} \end{bmatrix}. \tag{1.2.12}$$

In the exceptional case, when $\mathfrak{S}, B_c$ is one of the points $K_N$, both $\sigma_N^{+} = 0$ and $\sigma_{N+1}^{+} = 0$, while all the other eigenvalues have negative real parts. The expansion (1.2.9) is then given no longer by (1.2.12) but by

$$\begin{bmatrix} u_1 \\ \\ v_1 \end{bmatrix} = c_N^{+}(\tau)\begin{bmatrix} \sin N\pi r \\ \\ M_N^{+}\sin N\pi r \end{bmatrix} + c_{N+1}^{+}(\tau)\begin{bmatrix} \sin(N+1)\pi r \\ \\ M_{N+1}^{+}\sin(N+1)\pi r \end{bmatrix} + c_N^{-}(0)\exp(\sigma_N^{-}t)\begin{bmatrix} \phi_N^{-} \\ \\ \psi_N^{-} \end{bmatrix}$$

$$+ c_{N+1}^{-}(0)\exp(\sigma_{N+1}^{-}t)\begin{bmatrix} \phi_{N+1}^{-} \\ \\ \psi_{N+1}^{-} \end{bmatrix} + \mathrm{Re}\sum_{n\neq N,\, N+1} c_n^{\pm}(0)\exp(\sigma_n^{\pm}t)\begin{bmatrix} \phi_n^{\pm} \\ \\ \psi_n^{\pm} \end{bmatrix}. \tag{1.2.13}$$

Since $c_N^{+}(\tau)$ in the usual case, and $c_N^{+}(\tau)$ and $c_{N+1}^{+}(\tau)$ in the exceptional case, are not multiplied by decaying exponentials, their variation with $\tau$ is important. To find it we must look into (1.2.5) and (1.2.6). First we consider the usual case.

The functions $u_2$ and $v_2$ are assumed to be bounded, but for this to happen the right hand sides of (1.2.5) and (1.2.6) must satisfy a certain condition. To find it we take the inner product of the equations with $\hat{\underline{\phi}}_N^+$, integrate from t = 0 to t = T, divide by T and take the limit as $T \to \infty$. Terms involving $u_2$ and $v_2$ alone, and also exponentially decreasing terms, will vanish under this procedure. The integral for the remaining terms is

$$\int_0^T \int_0^1 \left\{ \sin^2 N\pi r \left[ -B'(0) \frac{dc_N^+}{d\tau} \left(1 - \frac{A^2}{B_c} (M_N^+)^2\right) + B'(0) c_N^+ \left(1 + \frac{A^2}{B_c} M_N^+\right)\right] \right.$$

$$\left. + \sin^3 N\pi r \, (c_N^+)^2 \left(\frac{B_c}{A} + 2AM_N^+\right)\left(1 + \frac{A^2}{B_c} M_N^+\right) \right\} dr\, dt \; .$$

(The signs of the coefficients of $\frac{dc_N^+}{d\tau}$, $c_N^+$, and $(c_N^+)^2$ are considered in the appendix. It is shown there that $1 - \frac{A^2}{B_c}(M_N^+)^2 > 0$, and $1 + \frac{A^2}{B_c} M_N^+ > 0$, but $\frac{B_c}{A} + 2AM_N^+$ may be of either sign.) We know that

$$\int_0^1 \sin^2 N\pi r \, dr = \frac{1}{2}$$

and

$$\int_0^1 \sin^3 N\pi r \, dr = \begin{cases} 0 & \text{if N is even} \\ \frac{4}{3N\pi} & \text{if N is odd} \end{cases} \; .$$

If N is odd, the condition that $u_2$ and $v_2$ be bounded is therefore

$$B'(0)\left(1 - \frac{A^2}{B_c}(M_N^+)^2\right) \frac{dc_N^+}{d\tau} = B'(0)\left(1 + \frac{A^2}{B_c} M_N^+\right) c_N^+$$

$$+ \frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)\left(1 + \frac{A^2}{B_c} M_N^+\right)(c_N^+)^2 \; . \qquad (1.2.14)$$

If N is even or if $\frac{B_c}{A} + 2AM_N^+ = 0$, the term in $(c_N^+)^2$ is absent, and in order to obtain bounded solutions to (1.2.12) it is necessary to pick $B'(0) = 0$. Then (1.2.14) is satisfied identically, and to obtain information about $c_N^+$ it is necessary to look into equations (1.2.7) and (1.2.8).

The solution to (1.2.14) in the case that N is odd and $\frac{B_c}{A} + 2AM_N^+ \neq 0$ is

$$c_N^+(\tau) = \frac{c_N^+(\infty)c_N^+(0)\exp\gamma\tau}{c_N^+(\infty) - c_N^+(0)[1-\exp\gamma\tau]} , \qquad (1.2.15)$$

where $c_N^+(0)$ is given by (1.2.10),

$$\gamma = \frac{1 + \frac{A^2}{B_c} M_N^+}{1 - \frac{A^2}{B_c}(M_N^+)^2} \qquad \text{and} \qquad c_N^+(\infty) = \frac{-B'(0)}{\frac{8}{3N\pi}(\frac{B_c}{A} + 2AM_N^+)} .$$

If $c_N^+(0)$ has the same sign as $c_N^+(\infty)$, then as $\tau \to \infty$, $c_N^+(\tau)$ tends to the constant limit $c_N^+(\infty)$, which does not otherwise depend on the initial conditions. If $c_N^+(0)$ and $c_N^+(\infty)$ have opposite signs, then $c_N^+(\tau)$ tends to infinity in a finite time $\tau_o$, which is the time at which the denominator of (1.2.15) vanishes.

We conclude that certain initial conditions do not tend to a non-uniform steady state of small amplitude; presumably they tend to a state of finite amplitude. If $c_N^+(0)$ and $c_N^+(\infty)$ do have the same sign, then the asymptotic expansion of the solution to (1.1.1) and (1.1.2) is

$$X \sim A + \frac{\varepsilon c_N^+(\infty) c_N^+(0) \exp\gamma(B-B_c)t}{c_N^+(\infty) - c_N^+(0)[1-\exp\gamma(B-B_c)t]} \sin N\pi r$$

$$+ \varepsilon c_N^-(0) \exp\sigma_N^- t \sin N\pi r$$

$$+ \varepsilon \operatorname{Re} \sum_{n \neq N} c_n^{\pm}(0) \exp\sigma_n^{\pm} t \sin n\pi r + O(\varepsilon^2) , \qquad (1.2.16)$$

$$Y \sim \frac{B_c}{A} + \frac{\varepsilon c_N^+(\infty) c_N^+(0) \exp\gamma (B-B_c)t}{c_N^+(\infty) - c_N^+(0)[1-\exp\gamma(B-B_c)t]} M_N^+ \sin N\pi r$$

$$+ \varepsilon c_N^-(0) \exp\sigma_N^- t \; M_N^+ \sin N\pi r$$

$$+ \varepsilon \operatorname{Re} \sum_{n \neq N} c_n^{\pm}(0) \exp\sigma_n^{\pm} t \; M_n^{\pm} \sin n\pi r + O(\varepsilon^2) . \qquad (1.2.17)$$

So far the value of $B'(0)$ has not been found, nor has $\varepsilon$ been determined. However, $B(\varepsilon)$ and $\varepsilon$ are related by $B-B_c = \varepsilon B'(0) + O(\varepsilon^2)$. One convenient way to normalize $\varepsilon$ is to demand that the inner product of the solution $[u, v]^t$ (where $X = A+u$, $Y = B/A + v$) with the adjoint eigenfunction $\hat{\underline{\phi}}_N^+$ be $\varepsilon$. Then $B'(0)$ is uniquely determined. Another way is merely to choose $B-B_c = \varepsilon$. In terms of this second normalization, we find that as $t \to \infty$ the solutions (1.2.16) and (1.2.17) tend to the steady state

$$X \sim A - \frac{(B-B_c)\sin N\pi r}{\frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)} + O\left((B-B_c)^2\right) \tag{1.2.18}$$

and

$$Y \sim \frac{B_c}{A} - \frac{(B-B_c)M_N^+ \sin N\pi r}{\frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)} + O\left((B-B_c)^2\right) . \tag{1.2.19}$$

The method of construction of the solution (1.2.18) and (1.2.19) shows that it is stable, since initial conditions starting near the steady state tend to it.

If B is slightly less than $B_c$, so that B'(0) is negative, it is possible to go through the same analysis as above and discover that there is a bifurcating steady state, given by (1.2.18) and (1.2.19), which is approached as $\tau = (B-B_c)t$ tends to $+\infty$. This steady state must therefore be unstable, as initial conditions starting near it tend away from it as t increases. (Note that $\tau$ tends to $+\infty$ as t tends to $-\infty$ in this case.)

These results are summarized in the bifurcation diagram, figure 1.2.1. The "amplitude" is the coefficient of $\sin N\pi r$ in (1.2.18). It may be positive or negative, depending on the sign of $\frac{B_c}{A} + 2AM_N^+$. The solid lines indicate stable branches, while the dotted lines indicate unstable branches.

When N is even it is necessary to find $c_N^+(\tau)$ by considering (1.2.7) and (1.2.8). The equations simplify somewhat since $B'(0) = 0$. Equations (1.2.5) and (1.2.6) become

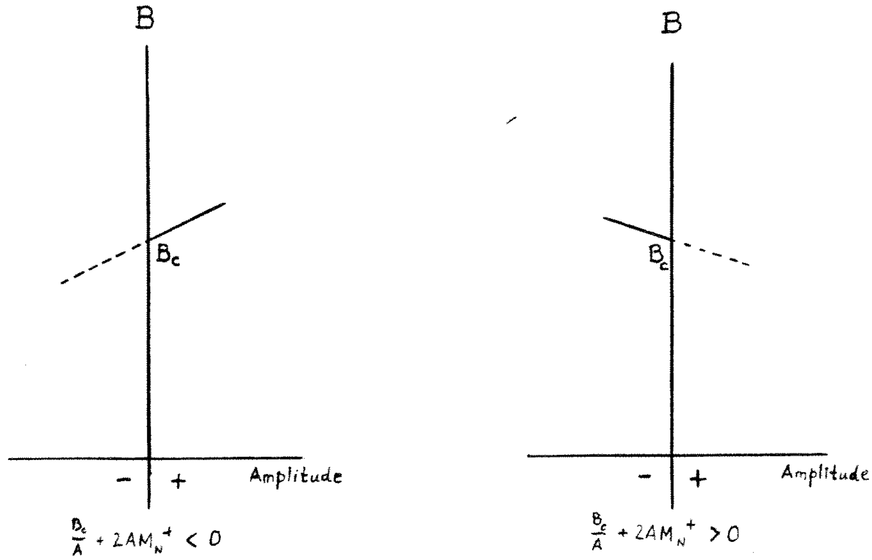


Figure 1.2.1. Bifurcation of a non-uniform steady state when N is odd.

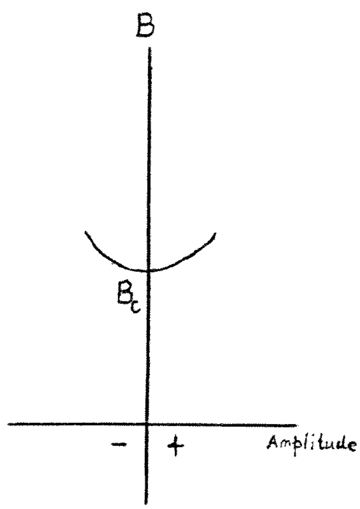


Figure 1.2.2. Bifurcation of a non-uniform steady state when N is even.

$$\frac{\partial u_2}{\partial t} = (B_c - 1)\, u_2 + A^2 v_2 + D\,\frac{\partial^2 u_2}{\partial r^2} + \frac{B_c}{A}\,(c_N^+(\tau)\sin N\pi r)^2$$
$$+ 2AM_N^+\,(c_N^+(\tau)\sin N\pi r)^2$$
$$+(\text{exponentially decaying terms}) \qquad (1.2.20)$$

and

$$\frac{\partial v_2}{\partial t} = -B_c u_2 - A^2 v_2 + \vartheta D\,\frac{\partial^2 v_2}{\partial r^2} - \frac{B_c}{A}(c_N^+(\tau)\sin N\pi r)^2$$
$$- 2A\overset{+}{MN}\,(c_N^+(\tau)\sin N\pi r)^2$$
$$+ (\text{exponentially decaying terms}). \qquad (1.2.21)$$

Hence

$$\begin{bmatrix} u_2 \\ \\ v_2 \end{bmatrix} = b_N^+(\tau)\begin{bmatrix} \sin N\pi r \\ \\ M_N^+ \sin N\pi r \end{bmatrix}$$
$$+ (c_N^+(\tau))^2 \sum_{n \neq N} \frac{(\frac{B_c}{A} + 2AM_N^+)(1 + \frac{A^2}{Bc} M_n^\pm)\int_0^1 \sin^2 N\pi r \sin n\pi r\, dr}{\frac{1}{2}\sigma_n^\pm\,(1 - \frac{A^2}{B_c}(M_n^\pm)^2)} \begin{bmatrix} \sin n\pi r \\ \\ M_n^\pm \sin n\pi r \end{bmatrix}$$
$$+ (\text{e.d.})\ .$$

Here $b_N^+(\tau)$ is an unknown function of $\tau$ and we have indicated exponentially decaying terms by the symbol (e. d. ). Let us denote the sum by $[\omega(r), \zeta(r)]^t$, so that

$$\begin{bmatrix} u_2 \\ \\ v_2 \end{bmatrix} = b_N^+(\tau) \begin{bmatrix} \sin N\pi r \\ \\ M_N^+ \sin N\pi r \end{bmatrix} + (c_N^+(\tau))^2 \begin{bmatrix} \omega(r) \\ \\ \zeta(r) \end{bmatrix} + (\text{e.d.}) \ . \qquad (1.2.22)$$

Using (1.2.12) and (1.2.22) in (1.2.7) and (1.2.8), we obtain

$$\frac{\partial u_3}{\partial t} = (B_c - 1)u_3 + A^2 v_3 + D \frac{\partial^2 u_3}{\partial r^2} - \frac{B''(0)}{2} \frac{dc_N^+}{d\tau} \sin N\pi r$$

$$+ \frac{B''(0)}{2} c_N^+ \sin N\pi r + (c_N^+)^3 M_N^+ \sin^3 N\pi r$$

$$+ 2A[(c_N^+)^3 \sin N\pi r(\zeta(r) + M_N^+ \omega(r)) + 2b_N^+ c_N^+ M_N^+ \sin^2 N\pi r]$$

$$+ \frac{2B_c}{A} \left[(c_N^+)^3 \sin N\pi r \ \omega(r) + b_N^+ c_N^+ \sin^2 N\pi r\right] + (\text{e.d.}) \ .$$

and

$$\frac{\partial v_3}{\partial \tau} = -B_c u_3 - A^2 v_3 + \vartheta D \frac{\partial^2 u_3}{\partial r^2} - \frac{B''(0)}{2} M_N^+ \frac{dc_N^+}{d\tau} \sin N\pi r$$

$$- \frac{B''(0)}{2} c_N^+ \sin N\pi r - (c_N^+)^3 M_N^+ \sin^3 N\pi r$$

$$-2A \left[(c_N^+)^3 \sin N\pi r(\zeta(r) + M_N^+ \omega(r)) + 2b_N^+ c_N^+ M_N^+ \sin^2 N\pi r\right]$$

$$- \frac{2B_c}{A} \left[(c_N^+)^3 \sin N\pi r \ \omega(r) + b_N^+ c_N^+ \sin^2 N\pi r\right] + (\text{e.d.}) \ .$$

Just as before, we take the inner product of these equations with $\hat{\underline{\phi}}_N^+$, integrate from $t = 0$ to $t = T$, divide by $T$, and take the limit as $T \to \infty$. Terms involving only $u_3$ and $v_3$, exponentially decreasing terms, and terms involving $\sin^3 N\pi r$ will vanish (this last because N is even so that $\int_0^1 \sin^3 N\pi r\,dr = 0$). What remains of the integral is

$$\int_0^T \int_0^1 \Big\{ \sin^2 N\pi r \Big[ -\frac{B''(0)}{2} \frac{dc_N^+}{d\tau} \left(1 - \frac{A^2}{B}(M_N^+)^2\right)$$

$$+ \frac{B''(0)}{2} c_N^+ \left(1 + \frac{A^2}{B} M_N^+\right)\Big] + \sin^4 N\pi r (c_N^+)^3 M_N^+ \left(1 + \frac{A^2}{B_c} M_N^+\right)$$

$$+ 2A \sin^2 N\pi r(\zeta(r) + M_N^+ \omega(r))\,(c_N^+)^3 \left(1 + \frac{A^2}{B_c} M_N^+\right)$$

$$+ \frac{2B_c}{A} \sin^2 N\pi r\, \omega(r)(c_N^+)^3 \left(1 + \frac{A^2}{B_c} M_N^+\right)\Big\} dr\,dt \ .$$

We know that $\int_0^1 \sin^4 N\pi r\,dr = \frac{3}{8}$, so the condition that $u_3$ and $v_3$ be bounded yields the following equation for $c_N^+(\tau)$:

$$\frac{B''(0)}{2} \cdot \frac{1 - \frac{A^2}{B_c}(M_N^+)^2}{1 + \frac{A^2}{B_c} M_N^+} \frac{dc_N^+}{d\tau} = \frac{B''(0)}{2} c_N^+$$

$$+ (c_N^+)^3 \Big\{ \frac{3}{4} M_N^+ + 4A \int_0^1 \sin^2 N\pi r(\zeta(r) + M_N^+ \omega(r))\,dr$$

$$+ \frac{4B_c}{A} \int_0^1 \sin^2 N\pi r\, \omega(r)\,dr \Big\} \ . \qquad (1.2.23)$$

The solution to (1.2.23) is

$$c_N^+(\tau) = \frac{|c_N^+(\infty)|\; c_N^+(0)\, e^{\gamma\tau}}{\{(c_N^+(0))^2(e^{2\gamma\tau} - 1) + (c_N^+(\infty))^2\}^{\frac{1}{2}}} \ ,$$

where

$$\gamma = \frac{1 + \frac{A^2}{B_c} M_N^+}{1 - \frac{A^2}{B_c} (M_N^+)^2} ,$$

$$c_N^+(\infty) = \pm \left(\frac{B''(0)}{2a}\right)^{\frac{1}{2}} \tag{1.2.24}$$

and $-a$ is the coefficient of $(c_N^+)^3$ in (1.2.23). (It can be shown that $\alpha > 0$.)

The choice of the square root in (1.2.24) requires a little care. Inspection of (1.2.23) shows that $\frac{dc_N^+}{d\tau}$ always has the same sign that it has initially. There are four cases: if $c_N^+(0) > |c_N^+(\infty)|$ or if $0 > c_N^+(0) > -|c_N^+(\infty)|$ then the slope is initially negative, while if $|c_N^+(\infty)| > c_N^+(0) > 0$ or $-|c_N^+(\infty)| > c_N^+(0)$ it is initially positive. Thus if $c_N^+(0) > 0$, $c_N^+(\tau)$ tends (monotonically) to $|c_N^+(\infty)|$, while if $c_N^+(0) < 0$, $c_N^+(\tau)$ tends to $-|c_N^+(\infty)|$. Thus the dependence of the steady state solution on the initial conditions is purely one of sign.

The asymptotic expansion of the solution to (1.1.1) and (1.1.2) in the case that N is even is therefore

$$X \sim A + \frac{\varepsilon\, |c_N^+(\infty)|\; c_N^+(0) \exp\gamma(B-B_c)t}{\left\{(c_N^+(0))^2(\exp 2\gamma\,(B-B_c)\,t-1)+(c_N^+(\infty))^2\right\}^{\frac{1}{2}}} \sin N\pi r$$

$$+ \varepsilon\; c_N^-(0) \exp\sigma_N^- \,t \sin N\pi r + \varepsilon \operatorname{Re} \sum_{n\neq N} c_n^{\pm}(0) \exp \sigma_n^{\pm} t \sin n\pi r$$

$$+ O(\varepsilon)^2 , \tag{1.2.25}$$

$$Y \sim \frac{B_c}{A} + \frac{\varepsilon \left| c_N^+(\infty) \right| c_N^+(0) \exp\gamma(B-B_c)t}{\{(c_N^+(0))^2(\exp 2\gamma(B-B_c)t-1)+(c_N^+(\infty))^2\}^{\frac{1}{2}}} M_N^+ \sin N\pi r$$

$$+ \varepsilon\, c_N^-(0) \exp \sigma_N^- t\, M_N^+ \sin N\pi r + \varepsilon \operatorname{Re} \sum_{n \neq N} c_n^\pm(0) \exp\sigma_n^\pm t\, M_n^\pm \sin n\pi r$$

$$+ O(\varepsilon^2) \qquad (1.2.26)$$

A convenient normalization of $\varepsilon$ is now $B-B_c = \varepsilon^2$. As $t \to \infty$, the solutions (1.2.25) and (1.2.26), valid when N is even and $\frac{B_c}{A} + 2AM_N^+ \neq 0$, tend to the steady state

$$X \sim A \pm \left(\frac{B-B_c}{a}\right)^{\frac{1}{2}} \sin N\pi r + O(B-B_c) , \qquad (1.2.27)$$

$$Y \sim \frac{B_c}{A} \pm \left(\frac{B-B_c}{a}\right)^{\frac{1}{2}} M_N^+ \sin N\pi r + O(B-B_c) . \qquad (1.2.28)$$

These results are summarized in the bifurcation diagram, figure 1.2.2. The bifurcating branches have been indicated by solid lines, since there is a range of initial conditions that tend to each of the steady states given by (1.2.27) and (1.2.28).

If $\frac{B_c}{A} + 2AM_N^+ = 0$, it is also necessary to pick $B'(0) = 0$ in order to prevent exponential growth of $c_N^+(\tau)$. Equations (1.2.5) and (1.2.6) in this case become

$$\frac{\partial u_2}{\partial t} = (B_c - 1)\, u_2 + A^2 v_2 + D \frac{\partial^2 u_2}{\partial r^2} + (\text{e.d.})$$

and
$$\frac{\partial v_2}{\partial t} = -B_c u_2 - A^2 v_2 + \vartheta D \frac{\partial^2 v_2}{\partial r^2} + (\text{e.d.}) ,$$

so that

$$\begin{bmatrix} u_2 \\ \\ v_2 \end{bmatrix} = b_N^+(\tau) \begin{bmatrix} \sin N\pi r \\ \\ M_N^+ \sin N\pi r \end{bmatrix} + (\text{e.d.}) \ .$$

Equations (1.2.7) and (1.2.8) are therefore

$$\frac{\partial u_3}{\partial t} = (B_c - 1)\, u_3 + A^2 v_3 + D \frac{\partial^2 u_3}{\partial r^2} - \frac{B''(0)}{2} \frac{dc_N^+}{d\tau} \sin N\pi r$$

$$+ \frac{B''(0)}{2} c_N^+ \sin N\pi r + (c_N^+)^3 M_N^+ \sin^3 N\pi r + (\text{e.d.})$$

and

$$\frac{\partial v_3}{\partial t} = -B_c u_3 - A^2 v_3 + \vartheta D \frac{\partial^2 v_3}{\partial r^2} - \frac{B''(0)}{2} \frac{dc_N^+}{d\tau} M_N^+ \sin N\pi r$$

$$- \frac{B''(0)}{2} c_N^+ \sin N\pi r - (c_N^+) M_N^+ \sin^3 N\pi r + (\text{e.d.}) \ .$$

In order that $u_3$ and $v_3$ be bounded, $c_N^+(\tau)$ must satisfy the differential equation

$$\frac{B''(0)}{2} \cdot \frac{1 - \frac{A^2}{B_c}(M_N^+)^2}{1 + \frac{A^2}{B_c} M_N^+} \frac{dc_N^+}{d\tau} = \frac{B''(0)}{2} c_N^+ + \frac{3}{4} M_N^+ (c_N^+)^3 \ . \tag{1.2.29}$$

As $\tau \to \infty$ the solution to (1.2.29) tends to one or the other of the steady states

$$c_N^+(\infty) = \pm \left( - \frac{2B''(0)}{3M_N^+} \right)^{\frac{1}{2}} \quad ,$$

depending on the sign of $c_N^+(0)$.

Next we consider the exceptional case when $\mathfrak{I}, B_c$ is one of the points $K_N$, so that $\sigma_N^+ = 0$ and $\sigma_{N+1}^+ = 0$. In order to find equations for $c_N^+(\tau)$ and $c_{N+1}^+(\tau)$, we substitute the expansion (1.2.13) into (1.2.5) and (1.2.6), take the inner product of the equations with $\hat{\underline{\phi}}_N^+$, integrate from $t = 0$ to $t = T$, divide by T and take the limit as $T \to \infty$, and then do the same thing taking the inner product of the equations with $\hat{\underline{\phi}}_{N+1}^+$. If N is odd, the resulting equations which $c_N^+(\tau)$ and $c_{N+1}^+(\tau)$ must satisfy in order that $u_2$ and $v_2$ be bounded are

$$B'(0)\left(1 - \frac{A^2}{B_c}(M_N^+)^2\right)\frac{dc_N^+}{d\tau} = B'(0)\left(1 + \frac{A^2}{B_c}M_N^+\right)c_N^+$$

$$+ \frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)\left(1 + \frac{A^2}{B_c}M_N^+\right)(c_N^+)^2$$

$$+ \frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]$$

$$\times\left(\frac{B_c}{A} + 2AM_{N+1}^+\right)\left(1 + \frac{A^2}{B_c}M_N^+\right)(c_{N+1}^+)^2 \qquad (1.2.30)$$

and

$$B'(0)\left(1 - \frac{A^2}{B_c}(M_{N+1}^+)^2\right)\frac{dc_{N+1}^+}{d\tau} = B'(0)\left(1 + \frac{A^2}{B_c}M_{N+1}^+\right)c_{N+1}^+$$

$$+ \frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]$$

$$\times\left(\frac{2B_c}{A} + 2A(M_N^+ + M_{N+1}^+)\right)\left(1 + \frac{A^2}{B_c}M_{N+1}^+\right)c_N^+ c_{N+1}^+ .$$

(1.2.31)

If N is even, the equations are

$$B'(0)\left(1-\frac{A^2}{B_c}(M_N^+)^2\right)\frac{dc_N^+}{d\tau} = B'(0)\,c_N^+\left(1+\frac{A^2}{B_c}M_N^+\right)$$

$$+\frac{1}{\pi}\left[\frac{1}{N-1}-\frac{1}{(3N+1)}\right]\left(\frac{2B_c}{A}+2A(M_N^+ + M_{N+1}^+)\right)\left(1+\frac{A^2}{B_c}M_N^+\right)c_N^+\,c_{N+1}^+$$

(1.2.32)

and

$$B'(0)\left(1-\frac{A^2}{B_c}(M_{N+1}^+)^2\right)\frac{dc_{N+1}^+}{d\tau} = B'(0)\,c_{N+1}^+\left(1+\frac{A^2}{B_c}M_{N+1}^+\right)$$

$$+\frac{8}{3(N+1)\pi}\left(\frac{B_c}{A}+2AM_{N+1}^+\right)\left(1+\frac{A^2}{B_c}M_{N+1}^+\right)(c_{N+1})^2$$

$$+\frac{1}{\pi}\left[\frac{1}{N-1}-\frac{1}{3N+1}\right]\left(\frac{B_c}{A}+2AM_N^+\right)\left(1+\frac{A^2}{B_c}M_{N+1}^+\right)(c_N^+)^2 \ .$$

(1.2.33)

We do not attempt to solve these equations explicitly. Instead we are satisfied with looking at the phase portraits of (1.2.30) and (1.2.31) and analyzing their critical points; this will provide all the relevant information about the steady states of (1.2.3) and (1.2.4) in the exceptional case being considered here. For the sake of definiteness it is assumed that $\frac{B_c}{A} + 2AM_N^+ > 0$ and $\frac{B_c}{A} + 2AM_N^+ > 0$, so that all the coefficients in (1.2.30) and (1.2.31) are positive. The phase trajectories in the $c_N^+$, $c_{N+1}^+$ plane are shown in figures 1.2.3 and 1.2.4. They are symmetric with respect to the $c_N^+$-axis. Examination of (1.2.31) shows that $c_{N+1}^+ = 0$ is a phase trajectory. Thus any trajectory beginning in the upper or lower half-plane must remain there.

The system may have four or two critical points, depending

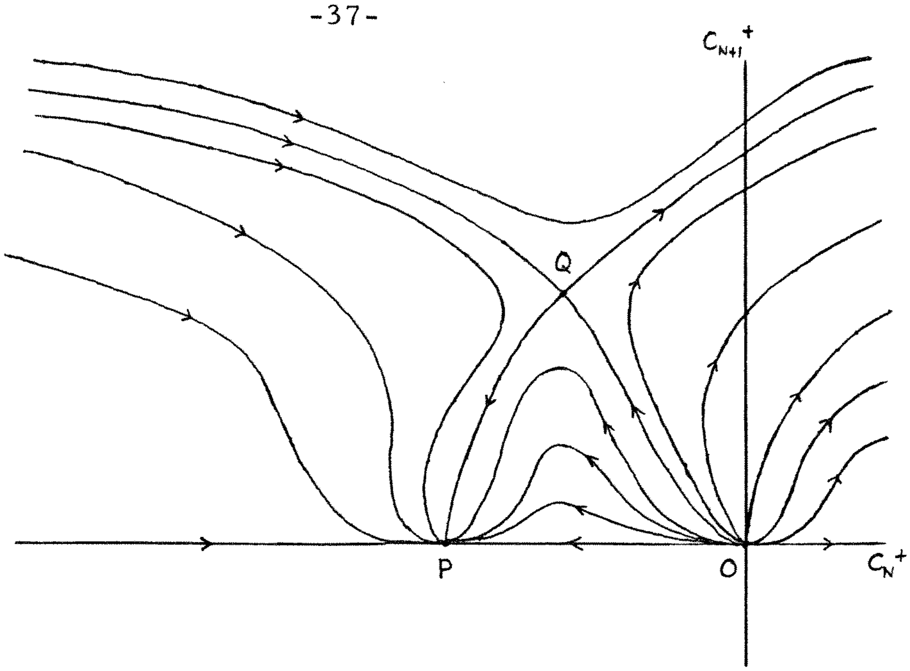


Figure 1.2.3. Phase trajectories of (1.2.30) and (1.2.31) when (1.2.34) is positive.

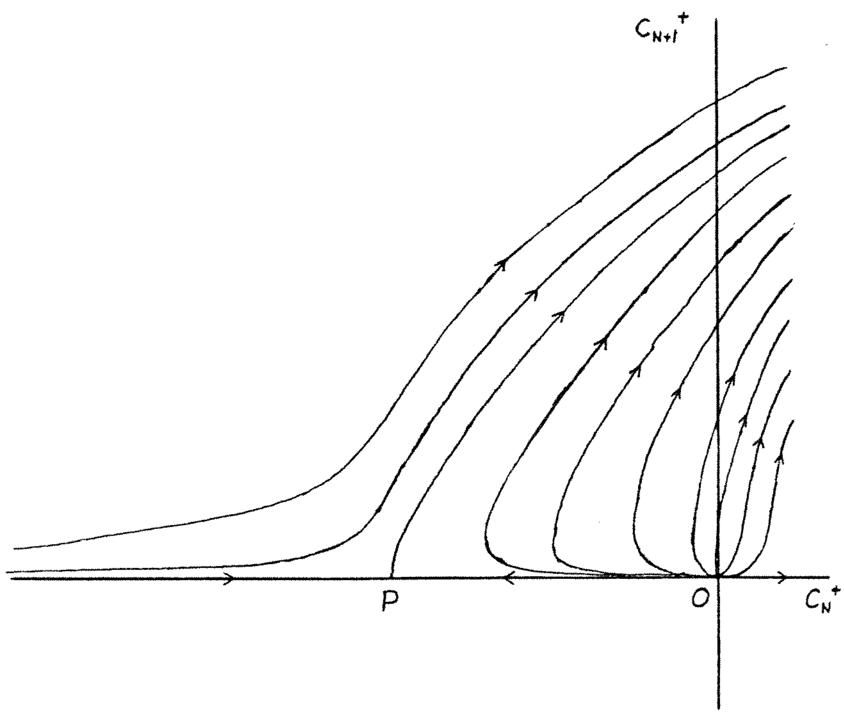


Figure 1.2.4. Phase trajectories of (1.2.30) and (1.2.31) when (1.2.34) is negative.

on the sign of the quantity

$$1 - \frac{\frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{B_c}{A} + 2A(M_N^+ + M_{N+1}^+)\right)} \qquad (1.2.34)$$

If it is positive, then there are four critical points O, P, Q, R; O is the origin and P, Q, and R are given by

P: $$c_N^+ = -\frac{B'(0)}{\frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)},$$

$$c_{N+1}^+ = 0 ;$$

Q: $$c_N^+ = \frac{-B'(0)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{2B_c}{A} + 2A(M_N^+ + M_{N+1}^+)\right)},$$

$$c_{N+1}^+ = \frac{B'(0)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{B_c}{A} + 2AM_{N+1}^+\right)}$$

$$\times \left\{1 - \frac{\frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^+\right)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{B_c}{A} + 2A(M_N^+ + M_{N+1}^+)\right)}\right\}^{\frac{1}{2}};$$

R: $$c_N^+ = \frac{-B'(0)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{B_c}{A} + 2A(M_N^+ + M_{N+1}^+)\right)},$$

$$c_{N+1}^{+} = \frac{-B'(0)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{B_c}{A} + 2AM_{N+1}^{+}\right)}$$

$$\times \left\{ 1 - \frac{\frac{8}{3N\pi}\left(\frac{B_c}{A} + 2AM_N^{+}\right)}{\frac{2}{\pi}\left[\frac{1}{N} + \frac{1}{2(N+2)} - \frac{1}{2(3N+2)}\right]\left(\frac{B_c}{A} + 2A(M_N^{+} + M_{N+1}^{+})\right)} \right\}^{\frac{1}{2}} .$$

Q and R are saddle points, O is an unstable nodal point, and P is a stable nodal point. If (1.2.34) is negative, then only O and P are critical points; O is an unstable nodal point and P is a saddle point. (The phase portraits for other signs of the coefficients, and for equations (1.2.32) and (1.2.33), are similar.)

It is seen that there are phase trajectories in both figures 1.2.3 and 1.2.4 that tend to infinity. Further, a solution represented by one of these trajectories tends to infinity in a finite time. This problem cannot be overcome by choosing B'(0) = 0 (as it could for the case N even), since (1.2.30) and (1.2.31) are not satisfied identically for that choice of B'(0). We conclude that there are initial conditions for (1.1.1) and (1.1.2) that do not tend to a new steady state of small amplitude in this case. Presumably they tend to a steady state of finite amplitude, which would be represented by a different branch of the bifurcation diagram.

Nicolis and Auchmuty [12] have also considered the bifurcation of non-uniform steady states for (1.1.1) and (1.1.2). However, their method does not consider the approach to these steady states in time, nor do they consider the exceptional case.

## 1.3 Multiple Steady States when Diffusion is Large

The results of the previous section are valid only when $\underline{\phi}_N^+$ is the sole eigenfunction that is excited or, in the exceptional case, when $\underline{\phi}_N^+$ and $\underline{\phi}_{N+1}^+$ are excited; the amplitude of the disturbance calculated is small. For the case $D_Y >> 1$ it is possible to find non-uniform steady states of finite amplitude. There is no restriction on the parameter B, but the calculation does not consider the time-dependent equations. Thus in this section we study the boundary value problem

$$0 = A - (B+1) X + X^2 Y + D \frac{d^2 X}{dr^2} , \qquad (1.3.1)$$

$$0 = BX - X^2 Y + \vartheta D \frac{d^2 Y}{dr^2} , \qquad (1.3.2)$$

$$X(0) = X(1) = A; \quad Y(0) = Y(1) = \frac{B}{A} . \qquad (1.3.3)$$

We assume that $\vartheta D >> 1$ and look for solutions with the asymptotic expansion

$$X \sim X_o + \frac{1}{\vartheta D} X_1 + \frac{1}{(\vartheta D)^2} X_2 + \dots ,$$
$$Y \sim Y_o + \frac{1}{\vartheta D} Y_1 + \frac{1}{(\vartheta D)^2} Y_2 + \dots .$$

Substitution of these expansions into (1.3.1), (1.3.2), and (1.3.3) yields the following hierarchy of equations and boundary conditions:

$$0 = A - (B+1) X_o + X_o^2 Y_o + D \frac{d^2 X_o}{dr^2} , \qquad (1.3.4)$$

$$X_o(0) = X_o(1) = A ; \qquad (1.3.5)$$

$$\frac{d^2 Y_o}{dr^2} = 0 \quad , \tag{1.3.6}$$

$$Y_o(0) = Y_o(1) = \frac{B}{A} \quad ; \tag{1.3.7}$$

$$0 = \left[-(B+1)+2X_oY_o\right] X_1 + X_o^2 Y_1 + D \frac{d^2 X_1}{dr^2} \quad , \tag{1.3.8}$$

$$X_1(0) = X_1(1) = 0 \; ; \tag{1.3.9}$$

$$0 = BX_o - X_o^2 Y_o + \frac{d^2 Y_1}{dr^2} \quad , \tag{1.3.10}$$

$$Y_1(0) = Y_1(1) = 0 \quad . \tag{1.3.11}$$

The solution of (1.3.6) and (1.3.7) is $Y_o \equiv \frac{B}{A}$. This value can be substituted into (1.3.4) to yield the following boundary value problem for $X_o$:

$$0 = A - (B+1)X_o + \frac{B}{A} X_o^2 + D \frac{d^2 X_o}{dr^2} \quad , \tag{1.3.12}$$

$$X_o(0) = X_o(1) = A \quad . \tag{1.3.5}$$

One solution is $X_o \equiv A$ but there will be others, depending on B and D. The solutions of equation (1.3.12) could be written in terms of elliptic functions since the non-linearity is only quadratic; however we find it more transparent to treat (1.3.12) and (1.3.5) directly.

Equation (1.3.12) can be written as a system:

$$D \frac{dX_o}{dr} = v \; ,$$

$$\frac{dv}{dr} = - \left(\frac{B}{A} X_o^2 - (B+1)\, X_o + A\right) .$$

The phase trajectories of the system are shown in figure 1.3.1. They are symmetric about the line v = 0. The points $X_o = A$, $v = 0$ and $X_o = \frac{A}{B}$, $v = 0$ are critical points. A solution of the boundary value problem (1.3.12) and (1.3.5) will correspond to a trajectory that starts on the line $X_o = A$ and returns to the same line after a "time of flight" of 1.

One integration of (1.3.12) yields

$$\tfrac{1}{2}D\left(\frac{dX_o}{dr}\right)^2 + \frac{B}{A}\left[\tfrac{1}{3}X_o^3 - \tfrac{1}{2}(B+1)\frac{A}{B}X_o^2 + \frac{A^2}{B}X_o\right] = \tfrac{1}{2}DE^2 ,$$

where

$$E = \left.\frac{dX_o}{dr}\right|_{r=0} .$$

Thus the concentric integral curves in the picture get larger as E increases. The critical point $X_o = A$, $v = 0$ corresponds to $E = 0$. The separatrix can be located by demanding that $X_o = \frac{A}{B}$ be a double root of the equation

$$\frac{B}{A}\left[\tfrac{1}{3}X_o^3 - \tfrac{1}{2}(B+1)\frac{A}{B}X_o^2 + \frac{A^2}{B}X_o\right] - \tfrac{1}{2}DE^2 = 0 . \qquad (1.3.13)$$

If the other root is called $\beta$, then (1.3.13) must be the same equation as

$$\tfrac{1}{3}\frac{B}{A}\left(X_o - \frac{A}{B}\right)^2 (X_o - \beta) = 0 .$$

It is found that this forces

$$\beta = A + \tfrac{1}{2}\left(A - \frac{A}{B}\right) = A + \frac{A}{B}(B-1) .$$

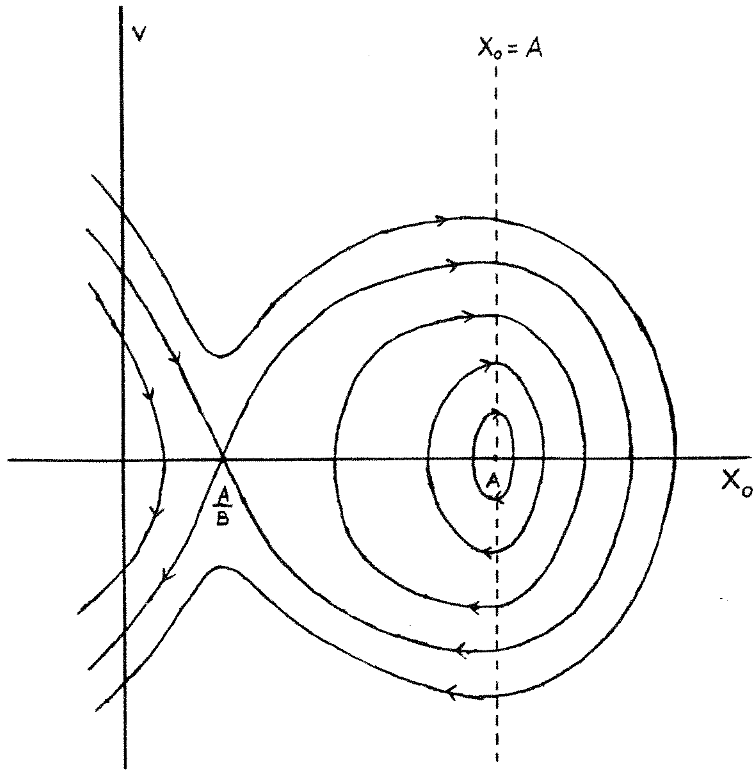


Figure 1.3.1. Phase trajectories of (1.3.12).

The value of E corresponding to the separatrix is $E_o$ where

$$E_o^2 = \frac{1}{3D} \frac{A^2(B-1)^3}{B^2} .$$

Aside from these distinguished trajectories, all other trajectories corresponding to a given value of E have either one or three intersections with the line v = 0, depending on whether $E > E_o$ or $E < E_o$. (The trajectories corresponding to $E < E_o$ have two branches, one of which is a closed curve inside the separatrix. The other is an unbounded curve which intersects v = 0 to the left of the critical point $X = \frac{A}{B}$, v = 0.) Choosing E is equivalent to choosing a particular trajectory; this can be done just as well by choosing a particular intersection of the trajectory with the line v = 0.

We now find it convenient to consider not $X_o$ and v but $u = X_o - A$ and v. The boundary value problem for u is

$$0 = (B-1)\,u + \frac{B}{A} u^2 + D \frac{d^2u}{dr^2} , \tag{1.3.14}$$

$$u(0) = u(1) = 0 . \tag{1.3.15}$$

This translation of the dependent variable merely shifts the phase portrait by an amount A to the left, and the critical point $X_o = A$, v = 0 to the origin. If now we call the intersections of a phase trajectory with the u-axis $\gamma$, $\alpha$, $\beta$ in increasing order (or just $\beta$ if $E > E_o$), then a particular choice of $\alpha$ also fixes $\gamma$, $\beta$, and E. It will always be true that when $E < E_o$,

$$\gamma < -\frac{A}{B}(B-1),$$

$$-\frac{A}{B}(B-1) < \alpha < 0 \quad ,$$

and $\quad \beta > 0 \quad .$

Further, as E tends to $E_o$ from 0, $\alpha$ tends monotonically from 0 to $-\frac{A}{B}(B-1)$. Conversely, as $\alpha$ tends to $-\frac{A}{B}(B-1)$ from 0, E tends monotonically from 0 to $E_o$ and $\beta$ tends monotonically from 0 to $\frac{1}{2}\frac{A}{B}(B-1)$. Thus we find it convenient to let $\alpha = -\mu\kappa$, where

$$\kappa = \frac{A}{B}(B-1) \quad ,$$

and $\mu$ is a parameter which can run from 0 to 1 when $\alpha$ is real.

A further integration of (1.3.14) gives

$$\pm \frac{du}{\left\{E^2 - \frac{2B}{AD}\left[\frac{1}{3}u^3 + \frac{A(B-1)}{2B}\;u^2\right]\right\}^{\frac{1}{2}}} = dr \; , \tag{1.3.16}$$

or

$$r = \pm \int_o^u \frac{du'}{\left\{\frac{2B}{3AD}\right\}^{\frac{1}{2}}\left\{(u'-\gamma)(u'-\alpha)(\beta-u')\right\}^{\frac{1}{2}}} \; . \tag{1.3.17}$$

This expression is valid when we integrate along portions of the closed trajectories. In order that (1.3.16) and (1.3.17) represent the same function, it is necessary that

$$-u^3 + (\gamma+\alpha+\beta)u^2 - (\alpha\beta+\alpha\gamma+\beta\gamma)u + \alpha\beta\gamma = -u^3 - \frac{3}{2}\frac{A}{B}(B-1) + \frac{3ADE^2}{2B} \; .$$

Substituting $\alpha = -\mu\kappa$, we find $\beta+\gamma = (-\frac{3}{2}+\mu)\kappa$ and $\beta\gamma = -\alpha(\beta+\gamma) = \mu(-\frac{3}{2}+\mu)\kappa^2$. These equations can be solved for $\beta$ and $\gamma$ in terms of $\mu$ and $\kappa$; the result is

$$\gamma = \tfrac{1}{2}\kappa\left\{-\frac{3}{2}+\mu-\left[(-\frac{3}{2}+\mu)^2-4\mu\,(-\frac{3}{2}+\mu)\right]^{\frac{1}{2}}\right\} \qquad (1.3.18)$$

and

$$\beta = \tfrac{1}{2}\kappa\left\{-\frac{3}{2}+\mu+\left[(-\frac{3}{2}+\mu)^2-4\mu\,(-\frac{3}{2}+\mu)\right]^{\frac{1}{2}}\right\} \quad . \qquad (1.3.19)$$

Of particular interest are the integrals

$$T_1(\mu) = 2\int_o^{\beta} \left(\frac{2B}{3AD}\right)^{-\frac{1}{2}} \left[(u-\gamma)(u-\alpha)(\beta-u)\right]^{-\frac{1}{2}} du$$

and

$$T_2(\mu) = 2\int_{\alpha}^{o} \left(\frac{2B}{3AD}\right)^{-\frac{1}{2}} \left[(u-\gamma)(u-\alpha)(\beta-u)\right]^{-\frac{1}{2}} du \ .$$

These represent the time of flight over half of a closed trajectory to the right and to the left of the line $u = 0$ respectively. Their sum $T(\mu)$ is the loop integral around the whole curve. (Even when $\gamma$ and $\alpha$ do not exist as real intersections, the integral $T_1(\mu)$ can be defined since the product $(u-\alpha)(u-\gamma)$ will be real.) The boundary value problem (1.3.14) and (1.3.15) will have a solution whenever there are values of $\mu$ such that any of the following occurs: $T_1(\mu) = 1$ or $T_2(\mu) = 1$; $T(\mu) = \frac{1}{n}$ for some integer n; or $nT_1(\mu) + (n \pm 1)\, T_2(\mu) = 1$ for some integer n. The number of possible solutions will depend on A, B, and D.

From (1.3.18) and (1.3.19) we obtain

$$T_2(\mu) = \left(\frac{6AD}{B}\right)^{\frac{1}{2}} \int_{-\mu\kappa}^{o} \left\{(u+\mu\kappa)\left[\mu(\tfrac{3}{2}-\mu)\kappa^2 - (\tfrac{3}{2}-\mu)\kappa u - u^2\right]\right\}^{-\frac{1}{2}} du$$

$$= \left(\frac{6AD}{B}\right)^{\frac{1}{2}} \int_{-1}^{o} \sqrt{\mu\kappa} \left\{(w+1)\left[\mu(\tfrac{3}{2}-\mu)\kappa^2 - (\tfrac{3}{2}-\mu)\mu\kappa^2 w - \mu^2\kappa^2 w^2\right]\right\}^{-\frac{1}{2}} dw$$

$$= \left(\frac{6AD}{B\kappa}\right)^{\frac{1}{2}} \int_{-1}^{o} \left\{(w+1)\left[(\tfrac{3}{2}-\mu) - (\tfrac{3}{2}-\mu)w - \mu w^2\right]\right\}^{-\frac{1}{2}} dw .$$

Thus

$$\frac{dT_2}{d\mu} = \left(\frac{6D}{B-1}\right)^{\frac{1}{2}} \int_{-1}^{o} \frac{\partial}{\partial\mu} \left\{(\tfrac{3}{2}-\mu) - (\tfrac{3}{2}-\mu)w - \mu w^2\right\}^{-\frac{1}{2}} \frac{dw}{\sqrt{1+w}}$$

$$= \left(\frac{6D}{B-1}\right)^{\frac{1}{2}} \int_{-1}^{o} \frac{1}{2} \frac{w^2 - w + 1}{\{(\frac{3}{2}-\mu) - (\frac{3}{2}-\mu)w - \mu w^2\}^{3/2}} \frac{dw}{\sqrt{1+w}}$$

$$= \left(\frac{D}{B-1}\right)^{\frac{1}{2}} \left(\frac{3}{2}\right)^{\frac{1}{2}} \int_{o}^{1} \frac{w^2 + w + 1}{\{(\frac{3}{2}-\mu) + (\frac{3}{2}-\mu)w - \mu w^2\}^{3/2}} \frac{dw}{\sqrt{1-w}} > 0 .$$

At $\mu = 0$ we have

$$\frac{dT_2}{d\mu} = \left(\frac{D}{B-1}\right)^{\frac{1}{2}} \cdot \frac{2}{3} \int_{o}^{1} \frac{(w^2+w+1)dw}{[(1+w)^3(1-w)]^{\frac{1}{2}}} .$$

The integral for $T_1(\mu)$ is most easily written in terms of $\beta = \nu\kappa$. Then

$$\frac{dT_1}{d\mu} = \frac{d\nu}{d\mu} \frac{dT_1}{d\nu} .$$

In terms of $\beta$, $(u-\gamma)(u-\alpha) = u^2 - (\alpha+\gamma)u + \alpha\gamma = u^2 + \kappa(\frac{3}{2}+\nu)u + \kappa^2\nu(\frac{3}{2}+\nu)$.

Thus

$$T_1(\mu) = \left(\frac{6AD}{B}\right)^{\frac{1}{2}} \int_o^{\nu\kappa} \left\{(\nu\kappa - u)\left[u^2 + \kappa(\tfrac{3}{2} + \nu)u + \kappa^2\nu(\tfrac{3}{2} + \nu)\right]\right\}^{-\frac{1}{2}} du$$

$$= \left(\frac{6AD}{B\kappa}\right)^{\frac{1}{2}} \int_o^1 \left\{(1-w)\left[\nu w^2 + (\tfrac{3}{2} + \nu)w + (\tfrac{3}{2} + \nu)\right]\right\}^{-\frac{1}{2}} dw \quad .$$

Hence from (1.3.19)

$$\frac{dT_1}{d\mu} = \left(\frac{6D}{B-1}\right)^{\frac{1}{2}} \cdot \tfrac{1}{2}\left[1 + \frac{\frac{3}{2} - 3\mu}{\sqrt{3(\frac{3}{2} - \mu)(\frac{1}{2} + \mu)}}\right] \times$$

$$\int_o^1 \frac{\partial}{\partial\nu}\left\{(\tfrac{3}{2} + \nu) + (\tfrac{3}{2} + \nu)w + \nu w^2\right\}^{-\frac{1}{2}} \frac{dw}{\sqrt{1-w}}$$

$$= \left(\frac{D}{B-1}\right)^{\frac{1}{2}} \cdot \tfrac{1}{2}\left[1 + \frac{\frac{3}{2} - 3\mu}{\sqrt{3(\frac{3}{2} - \mu)(\frac{1}{2} + \mu)}}\right]$$

$$\cdot - (\tfrac{3}{2})^{\frac{1}{2}} \int_o^1 \frac{w^2 + w + 1}{\{(\frac{3}{2} + \nu) + (\frac{3}{2} + \nu)w + \nu w^2\}^{3/2}} \frac{dw}{\sqrt{1-w}} < 0 \quad .$$

At $\mu = 0$, $\nu = 0$ as well and

$$\frac{dT_1}{d\mu} = -\left(\frac{D}{B-1}\right)^{\frac{1}{2}} \cdot \frac{2}{3} \int_o^1 \frac{(w^2+w+1)dw}{[(1+w)^3(1-w)]^{\frac{1}{2}}} \quad .$$

Thus at $\mu = 0$

$$\frac{d}{d\mu}(T_1 + T_2) = 0 \quad ,$$

$$\frac{d}{d\mu}(n(T_1+T_2)+T_1) < 0 \quad ,$$

and

$$\frac{d}{d\mu}\left(n(T_1+T_2)+T_2\right) > 0 \quad .$$

On the other hand, it is true that $\frac{dT}{d\mu} > 0$ for $\mu > 0$. This is most easily seen by considering

$$T(\mu) = \left(\frac{6D}{B-1}\right)^{\frac{1}{2}} \int_0^1 (1-w)^{-\frac{1}{2}} \left[\left\{\frac{3}{2} - \mu + (\frac{3}{2} - \mu)w - \mu w^2\right\}^{\frac{1}{2}} \right.$$

$$\left. + \left\{\frac{3}{2} + \nu + (\frac{3}{2} + \nu)\, w + \nu w^2\right\}^{\frac{1}{2}}\right]^{-1} dw \ .$$

It can be shown that $\frac{d\nu}{d\mu} \leqslant 1$ and $\frac{1}{2}\mu \leqslant \nu \leqslant \mu$. It follows that the term in brackets in the integrand is a decreasing function of $\mu$, so that the integrand is an increasing function of $\mu$.

Next we wish to make estimates on $T_1(\mu)$ and $T_2(\mu)$. It is possible to evaluate $T_1(0)$ and $T_2(0)$: for $\mu = 0$ equation (1.3.14) is linear, namely

$$D\,\frac{d^2u}{dr^2} + (B-1)\,u = 0 \quad . \tag{1.3.20}$$

Thus $u = c \sin \omega r$, where

$$\omega = \left(\frac{B-1}{D}\right)^{\frac{1}{2}} \quad . \tag{1.3.21}$$

Hence $T_1(0) = T_2(0) = \frac{\pi}{\omega}$, and $T(0) = \frac{2\pi}{\omega}$. (This could also be seen from the integrals.)

We had

$$T_1(\mu) = \left(\frac{6D}{B-1}\right)^{\frac{1}{2}} \int_0^1 \left\{(1-w)\left[\nu w^2 + (\frac{3}{2} + \nu)w + (\frac{3}{2} + \nu)\right]\right\}^{-\frac{1}{2}} dw \quad .$$

But in the range $0 \leqslant w \leqslant 1$,

$$\nu w^2 + (\tfrac{3}{2} + \nu)w + (\tfrac{3}{2} + \nu) \geqslant (\tfrac{3}{2} + \nu) + (\tfrac{3}{2} + \nu)w = (\tfrac{3}{2} + \nu)(1+w) .$$

Thus

$$T_1(\mu) \leqslant \left(\frac{6D}{B-1}\right)^{\frac{1}{2}} (\tfrac{3}{2} + \nu)^{-\frac{1}{2}} \int_0^1 \frac{dw}{[1-w^2]^{\frac{1}{2}}}$$

$$= \frac{\pi}{\omega} \left(\frac{1}{1+\frac{2}{3}\nu}\right)^{\frac{1}{2}} .$$

The integral $T_1$ always exists as $\beta = \nu\kappa$ tends to infinity, and the above calculation shows that it tends to zero.

Also,

$$T_2(\mu) = \frac{\sqrt{6}}{\omega} \int_{-1}^{0} \left\{(w+1)\left[(\tfrac{3}{2} - \mu) - (\tfrac{3}{2} - \mu)w - \mu w^2\right]\right\}^{-\frac{1}{2}} dw .$$

But for $0 \leqslant w \leqslant 1$

$$\tfrac{3}{2} - \mu - (\tfrac{3}{2} - \mu)w - \mu w^2 \leqslant 3 - 3\mu + (3\mu - \tfrac{3}{2})(w+1) .$$

Thus for $\mu$ sufficiently close to 1,

$$T_2(\mu) \geqslant \frac{\sqrt{6}}{\omega} (3\mu - \tfrac{3}{2})^{-\frac{1}{2}} \int_{-1}^{0} \frac{dw}{\left\{(1+w)\left[\frac{1-\mu}{\mu-\frac{1}{2}} + 1 + w\right]\right\}^{\frac{1}{2}}}$$

$$= \frac{1}{\omega} \frac{2}{(2\mu-1)^{\frac{1}{2}}} \int_{-1}^{0} \frac{dw}{\left\{(w + \frac{\mu}{2\mu-1})^2 - \frac{(1-\mu)^2}{(2\mu-1)^2}\right\}^{\frac{1}{2}}}$$

$$= \frac{1}{\omega} \frac{2}{(2\mu-1)^{\frac{1}{2}}} \int_{\frac{1-\mu}{2\mu-1}}^{\frac{\mu}{2\mu-1}} \frac{dz}{\left\{z^2 - (\frac{1-\mu}{2\mu-1})^2\right\}^{\frac{1}{2}}}$$

$$= \frac{1}{\omega} \frac{2}{(2\mu-1)^{\frac{1}{2}}} \text{ arg cosh } \frac{\mu}{1-\mu} .$$

Thus $T_2(\mu)$ tends to infinity as $\mu$ tends to 1, and at least as fast as $|\log(1-\mu)|$.

We can now determine the number and form of the solutions to the boundary value problem (1.3.14) and (1.3.15). The results are summarized in the bifurcation diagram, figure 1.3.2. On it we have plotted T versus $\mu$. The curves represent nT, $nT+T_1$, and $nT+T_2$ as functions of $\mu$. All except $T_1(\mu)$ asymptote to $\mu = 1$. Curves to the left of the T-axis correspond to branches nT or $nT+T_2$, for which $\left.\frac{du}{dr}\right|_{r=0} < 0$, while curves to the right of the T-axis correspond to branches nT or $nT+T_1$, for which $\left.\frac{du}{dr}\right|_{r=0} > 0$. There will be solutions of (1.3.12) and (1.3.5) whenever one of these curves intersects the horizontal line T = 1. The number of solutions therefore depends strongly on the value of $\frac{\pi}{\omega}$. For the example shown in figure 1.3.2, there are exactly five solutions to the boundary value problem. Figure 1.3.3 sketches them. It is seen that solutions corresponding to larger values of $\mu$ (and hence larger amplitudes) have fewer internal zeroes and larger initial gradients. Solutions of the form $nT+T_1$ or $nT+T_2$ are symmetric with respect to $r = \frac{1}{2}$.

If we substitute any of the multiple solutions to (1.3.12) and (1.3.5) into (1.3.8), (1.3.9) and (1.3.10), (1.3.11), we obtain unique solutions to these boundary value problems. Thus consideration of the next order does not affect the multiplicity of solutions to (1.3.1), (1.3.2), and (1.3.3) in this limit.

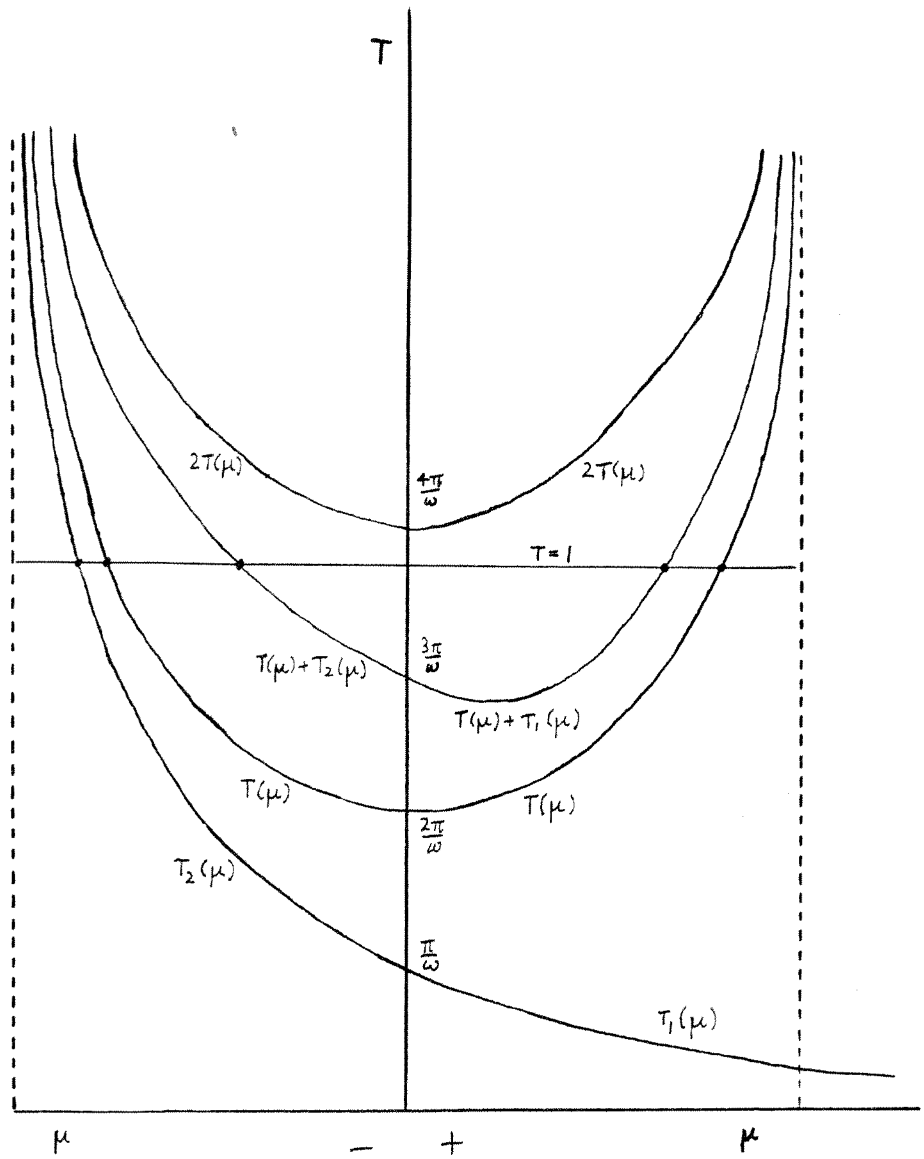


Figure 1. 3. 2. Bifurcation diagram for non-uniform steady states. If $\frac{\pi}{\omega} = \frac{4}{15}$ there are exactly five non-trivial solutions indicated by the dots. The three to the left of the T-axis have negative initial slope; the other two have positive initial slope.

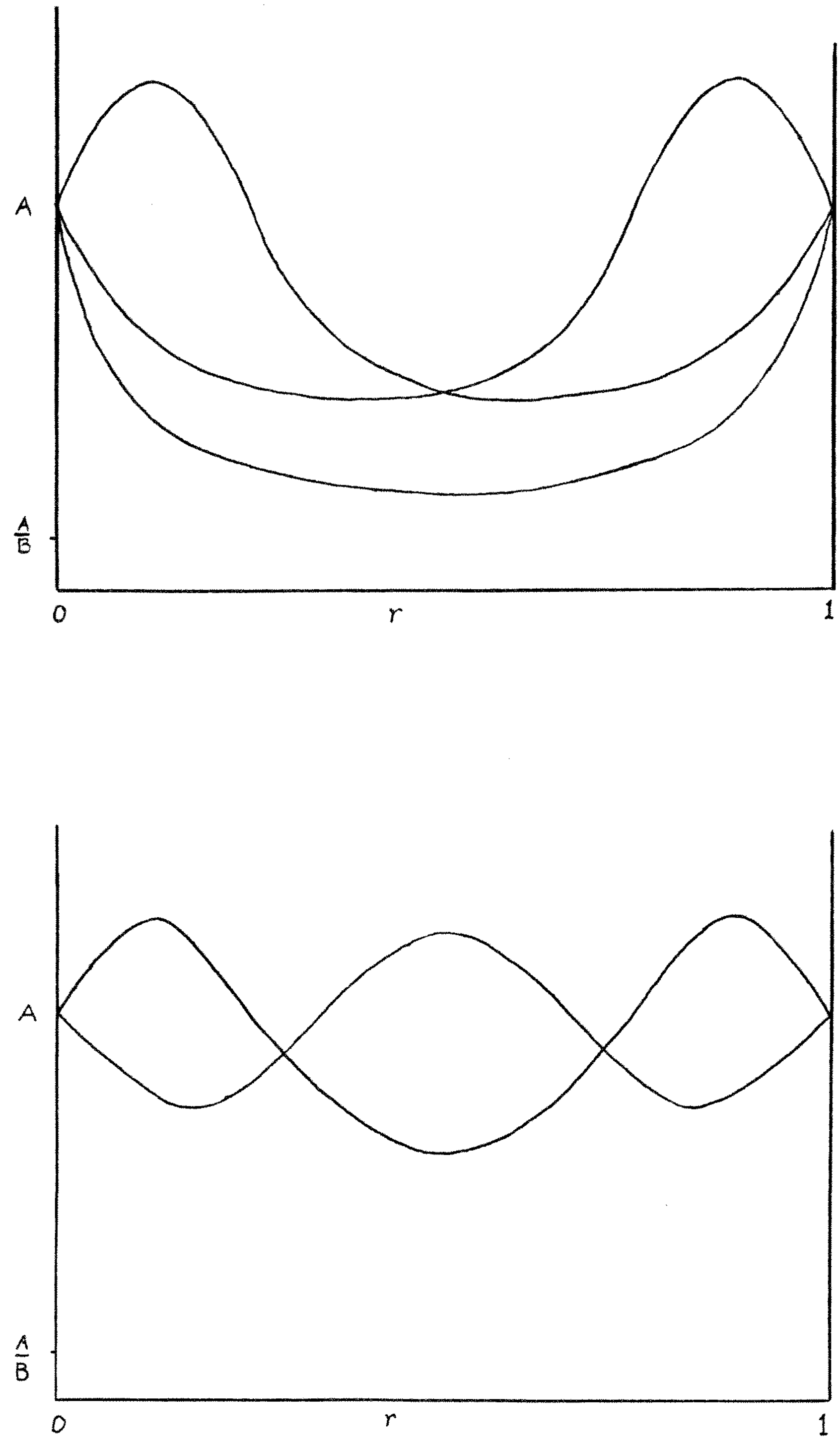


Figure 1. 3. 3. Sketches of the five non-uniform steady states found when $\frac{\pi}{\omega} = \frac{4}{15}$.

The bifurcation diagram 1.3.2, which indicates non-uniform steady states of finite amplitude in the limit $\delta \to \infty$, should be compared with the bifurcation diagrams 1.2.1 and 1.2.2 found by perturbation techniques. From it one can make a plausible guess as to how figures 1.2.1 and 1.2.2 are to be extended to finite amplitude disturbances. Branches of the form nT correspond to N even in the notation of section 1.2, while branches of the form $nT+T_1$ or $nT+T_2$ correspond to N odd. It is reasonable to predict that the bifurcating branches of figures 1.2.1 and 1.2.2 extend to curves like $nT+T_1$ (or $nT+T_2$) and nT, respectively. In particular, the subcritical branch of figure 1.2.1, indicated by the dotted line, eventually curves back. It can further be predicted that the branches asymptote to some vertical line, so that the amplitude of any non-uniform steady state (no matter what the value of B may be) is uniformly bounded.

## 1.4 Bifurcation of Periodic Solutions

In this section we wish to consider solutions of (1.1.1) and (1.1.2) when the uniform state is unstable and the point $\vartheta$, B is only slightly above the neutral stability curve in region III of figure 1.1.3. It will be shown by use of the two-timing technique that the solutions tend to a time-periodic function of small amplitude. Again we follow the analysis of Kogelman and Keller [5].

As in section 1.2, the equations to be studied are (1.2.3) - (1.2.8), and the solution of (1.2.3) and (1.2.4) is given by (1.2.9). However, now $B_c = 1+A^2 + \pi^2 D(1+\vartheta)$, and the eigenvalues with the greatest real parts are $\sigma_1^+$ and $\sigma_1^-$. Specifically,

$$\sigma_1^{\pm}(B_c) = \pm\, i \left\{4A^2 B_c - \left[B_c - 1 + A^2 + \pi^2 D(\vartheta - 1)\right]^2\right\}^{\frac{1}{2}}, \qquad (1.4.1)$$

and all other eigenvalues have negative real parts. The expansion (1.2.9) therefore becomes

$$\begin{bmatrix} u_1 \\ \\ v_1 \end{bmatrix} = \mathrm{Re} \quad c_1^+(\tau)\, e^{it\alpha} \begin{bmatrix} \phi_1^+ \\ \\ \psi_1^+ \end{bmatrix} + c_1^-(\tau)\, e^{-it\alpha} \begin{bmatrix} \phi_1^- \\ \\ \psi_1^- \end{bmatrix} + (\text{e.d.}),$$

where $\alpha = \mathrm{Im}\, \sigma_1^+$ and (e.d.) indicates exponentially decreasing terms. Since in this case $M_1^- = \overline{M_1^+}$, we can write the real part as

$$\begin{bmatrix} u_1 \\ \\ v_1 \end{bmatrix} = c_1(\tau)\, e^{it\alpha}\, \underline{\phi}^+ + \overline{c_1(\tau)}\, e^{-it\alpha}\, \overline{\underline{\phi}_1^+} + (\text{e.d.})\,, \qquad (1.4.2)$$

where $c_1 = \frac{1}{2}(\overline{c_1^+ + c_1^-})$. From (1.2.10) and (1.2.11), the initial condition on $c_1$ is

$$c_1(0) = \frac{2\int_0^1 \{h_\varepsilon(r,0) - \frac{A^2}{B_c} M_1^+ \; k_\varepsilon(r,0)\} \sin \pi r dr}{1 - \frac{A^2}{B_c} (\overline{M_1^+})^2} \qquad (1.4.3)$$

Substitution of the expansion (1.4.2) into (1.2.5) and (1.2.6) yields

$$\frac{\partial u_2}{\partial t} = (B_c - 1)u_2 + A^2 v_2 + D \frac{\partial^2 u_2}{\partial r^2} - B'(0) \sin \pi r \left[c_1' e^{ita} + \overline{c_1'} e^{-ita}\right]$$

$$+B'(0) \sin \pi r \left[c_1 e^{ita} + \overline{c}_1 e^{-ita}\right]$$

$$+ \frac{B_c}{A} \sin^2 \pi r \left[c_1^2 e^{2ita} + 2|c_1|^2 + \overline{c}_1^2 e^{-2ita}\right]$$

$$+2A \sin^2 \pi r \left[M_1^+ c_1^2 e^{2ita} + M_1^+ |c_1|^2 + \overline{M_1^+} |c_1|^2 + \overline{M_1^+} \overline{c}_1^2 e^{-2ita}\right] + (\text{e.d.}),$$

(1.4.4)

$$\frac{\partial v_2}{\partial t} = -B_c u_2 - A^2 v^2 + \vartheta D \frac{\partial^2 v_2}{\partial r^2}$$

$$-B'(0) \sin \pi r \left[M_1^+ c_1' e^{ita} + \overline{M_1^+} \overline{c_1'} e^{-ita}\right]$$

$$-B'(0) \sin \pi r \left[c_1 e^{ita} + \overline{c}_1 e^{-ita}\right] - \frac{B_c}{A} \sin^2 \pi r \left[c_1^2 e^{2ita} + 2|c_1|^2 + \overline{c}_1^2 e^{-2ita}\right]$$

$$-2A \sin^2 \pi r \left[M_1^+ c_1^2 e^{2ita} + M_1^+ |c_1|^2 + \overline{M_1^+} |c_1|^2 + \overline{M_1^+} \overline{c}_1^2 e^{-2ita}\right] + (\text{e.d.}).$$

(1.4.5)

We take the inner product of these equations with $\hat{\underline{\phi}}_1^+$, multiply by $e^{it\alpha}\, T^{-1}$, integrate from 0 to T, and take the limit as $T \to \infty$. Terms involving only $u_2$ and $v_2$ drop out, since $u_2$ and $v_2$ are assumed bounded; so do exponentially decreasing terms. There will also arise terms of the form

$$\int_0^T e^{ijt\alpha} f(\tau)\, dt \,,$$

where j = 3, 1, -1. Since functions $f(\tau)$ change only slowly in comparison with the rapid oscillations of $e^{ijt\alpha}$, the integral is o(T). Thus terms of this type disappear in the limiting procedure. The only remaining term in the integral is

$$\int_0^T \int_0^1 \sin^2 \pi r \left[ -B'(0) \frac{d\bar{c}_1}{d\tau} \left( 1 - \frac{A^2}{B_c} (M_1^+)^2 \right) \right.$$
$$\left. + B'(0)\, \bar{c}_1 \left( 1 + \frac{A^2}{B_c} M_1^+ \right) \right] dr\, dt \;.$$

In order that $u_1$ and $v_1$ be bounded it will be necessary to pick $B'(0) = 0$, and to look into (1.2.7) and (1.2.8) to find an equation for $c_1(\tau)$.

The solution of (1.4.4) and (1.4.5) is

$$\begin{bmatrix} u_2 \\ \\ v_2 \end{bmatrix} = b_1(\tau)\, e^{it\alpha} \begin{bmatrix} \sin \pi r \\ \\ M_1^+ \sin \pi r \end{bmatrix} + \overline{b_1(\tau)}\, e^{-it\alpha} \begin{bmatrix} \sin \pi r \\ \\ \overline{M_1^+} \sin \pi r \end{bmatrix}$$
$$+ c_1^2\, e^{2it\alpha} \sum_{n=2}^{\infty} \int_0^1 \sin^2 \pi r \sin n\pi r\, dr \left( \frac{B_c}{A} + 2AM_1^+ \right) \frac{\rho_n^{\pm}}{\sigma_n^{\pm}}\, \underline{\phi}_n^{\pm}$$
$$+ |c_1|^2 \sum_{n=2}^{\infty} \int_0^1 \sin^2 \pi r \sin n\pi r\, dr \left( 2\frac{B_c}{A} + 2A(M_1^+ + \overline{M_1^+}) \right) \frac{\rho_n^{\pm}}{\sigma_n^{\pm}}\, \underline{\phi}_n^{\pm}$$

$$+ \bar{c}_1^2 e^{-2it\alpha} \sum_{n=2}^{\infty} \int_0^1 \sin^2 \pi r \sin n\pi r \, dr \; \frac{B_c}{A} + 2A\overline{M_1^+} \; \frac{\rho_n^{\pm}}{\sigma_n^{\pm}} \underline{\phi}_n^{\pm} + (\text{e.d.}),$$

where $b_1(\tau)$ is an undetermined function and

$$\rho_n^{\pm} = 2 \; \frac{1 + \frac{A^2}{B_c} \overline{M_n^{\pm}}}{1 - \frac{A^2}{B_c} (M_n^{\pm})^2} \; .$$

If $M_n^+$ is complex, then $M_n^- = \overline{M_n^+}$. Thus if $M_n^+$ is complex,

$$\overline{\frac{\rho_n^+}{\sigma_n^+} \underline{\phi}_n^+} = \frac{\rho_n^-}{\sigma_n^-} \underline{\phi}_n^- \; ,$$

so that the sum

$$\sum_{n=2}^{\infty} \int_0^1 \sin^2 \pi r \sin n\pi r \, dr \; \frac{\rho_n^{\pm}}{\sigma_n^{\pm}} \underline{\phi}_n^{\pm}$$

is always real. If we define $\underline{w}(r) = [w(r), z(r)]^t$ by

$$\underline{w}(r) = \left(\frac{B_c}{A} + 2AM_1^+\right) \sum_{n=2}^{\infty} \int_0^1 \sin^2 \pi r \sin n\pi r \, dr \; \frac{\rho_n^{\pm}}{\sigma_n^{\pm}} \underline{\phi}_n^{\pm} \; ,$$

then the solution of (1.4.4) and (1.4.5) is given by

$$\begin{bmatrix} u_2 \\ v_2 \end{bmatrix} = b_1(\tau) e^{it\alpha} \begin{bmatrix} \sin \pi r \\ M_1^+ \sin \pi r \end{bmatrix} + \overline{b_1(\tau)} \, e^{-it\alpha} \begin{bmatrix} \sin \pi r \\ \overline{M_1^+} \sin \pi r \end{bmatrix} \qquad (1.4.6)$$

$$+ c_1^2 e^{2it\alpha} \underline{w} + |c_1|^2 (\underline{w} + \overline{\underline{w}}) + \bar{c}_1^2 e^{-2it\alpha} \overline{\underline{w}} + (\text{e.d.}) \; .$$

We substitute (1.4.2) and (1.4.6) into (1.2.7) and (1.2.8) to obtain

$$\frac{\partial u_3}{\partial t} = (B_c - 1)\, u_3 + A^2 v_3 + D\,\frac{\partial^2 u_3}{\partial r^2} + \frac{B''(0)}{2}$$

$$\times \left[ -\frac{dc_1}{d\tau}\, e^{it\alpha} - \frac{d\bar{c}_1}{d\tau}\, e^{-it\alpha} + c_1\, e^{it\alpha} + \bar{c}_1\, e^{-it\alpha} \right] \sin\pi r$$

$$+ \sin^3\pi r\, [c_1^3\, e^{3it\alpha}\, M_1^+ + 3|c_1|^2\, c_1\, e^{it\alpha}\, M_1^+$$

$$+ 3|c_1|^2\, \bar{c}_1\, e^{-it\alpha}\, \overline{M_1^+} + \bar{c}_1^3\, e^{-3it\alpha}\, \overline{M_1^+}\,]$$

$$+ 2A \sin^2\pi r\, [2b_1 c_1\, M_1^+\, e^{2it\alpha}$$

$$+ (b_1\bar{c}_1 + \bar{b}_1 c_1)(M_1^+ + \overline{M_1^+}) + 2\,\overline{b_1 c_1}\, e^{-2it\alpha}\, \overline{M_1^+}\,]$$

$$+2A\ z(r) \sin\pi r\, [c_1^3\, e^{3it\alpha} + |c_1|^2\, c_1\, e^{it\alpha}]$$

$$+2A(z+\bar{z})\sin\pi r\, [|c_1|^2\, c_1\, e^{it\alpha} + |c_1|^2\, \bar{c}_1\, e^{-it\alpha}]$$

$$+2A\bar{z}\ \sin\pi r\, [|c_1|^2\, \bar{c}_1\, e^{-it\alpha} + \bar{c}_1^3\, e^{-3it\alpha}]$$

$$+2Aw(r)\ \sin\pi r\, [c_1^3\, e^{3it\alpha}\, M_1^+ + |c_1|^2\, c_1\, e^{it\alpha}\, \overline{M_1^+}]$$

$$+2A(w+\bar{w})\sin\pi r\, [|c_1|^2\, c_1\, e^{it\alpha}\, M_1^+ + |c_1|^2 \bar{c}_1\, e^{-it\alpha}\, \overline{M_1^+}]$$

$$+2A\ \bar{w}\ \sin\pi r\, [\bar{c}_1^3\, e^{-3it\alpha}\, \overline{M_1^+} + |c_1|^2\, \bar{c}_1\, e^{-it\alpha}\, M_1^+]$$

$$+ \frac{2B_c}{A} \sin^3 \pi r \left[ b_1 c_1 e^{2it\alpha} + (\bar{b}_1 c_1 + b_1 \bar{c}_1) + \overline{b_1 c_1}\, e^{-2it\alpha} \right]$$

$$+ \frac{2B_c}{A} w \sin \pi r \left[ c_1^3 e^{3it\alpha} + |c_1|^2 c_1 e^{it\alpha} \right]$$

$$+ \frac{2B_c}{A} (w+\bar{w}) \sin \pi r \left[ |c_1|^2 c_1 e^{it\alpha} + |c_1|^2 \bar{c}_1 e^{-it\alpha} \right]$$

$$+ \frac{2B_c}{A} \bar{w} \sin \pi r \left[ \bar{c}_1^3 e^{-3it\alpha} + |c_1|^2 \bar{c}_1 e^{-it\alpha} \right] + (\text{e.d.})$$

and

$$\frac{\partial v_3}{\partial t} = -B_c u_3 - A^2 v_3 + \vartheta D \frac{\partial^2 v_3}{\partial r^2} + \frac{B''(0)}{2}$$

$$\times \left[ -M_1^+ \frac{dc_1}{d\tau} e^{it\alpha} - M_1^+ \frac{d\bar{c}_1}{d\tau} e^{-it\alpha} + c_1 e^{it\alpha} + \bar{c}_1 e^{-it\alpha} \right] \sin \pi r$$

$$- f(r) + (\text{e.d.}) ,$$

where $f(r)$ is the remaining part of the inhomogeneous portion of the right hand side of the previous equation. To find an equation for $c_1$ we take the inner product of these equations with $\hat{\underline{\phi}}_1^+$, multiply by $T^{-1} e^{it\alpha}$, integrate from $t = 0$ to $t = T$, and take the limit as $T \rightarrow \infty$. Since $u_3$ and $v_3$ are assumed bounded, there results in the same manner as before the following equation:

$$0 = -\tfrac{1}{2}\left(1 - \frac{A^2}{B_c}(M_1^+)^2\right) \frac{B''(0)}{2} \frac{d\bar{c}_1}{d\tau} + \tfrac{1}{2}\left(1 + \frac{A^2}{B_c} M_1^+\right) \frac{B''(0)}{2} \bar{c}_1$$

$$+ |c_1|^2 \bar{c}_1 \left(1 + \frac{A^2}{B_c} M_1^+\right) \left\{ \frac{9}{8} M_1^+ + 2A \int_0^1 \sin^2 \pi r (z + 2\bar{z})\, dr \right.$$

$$+ \frac{2B_c}{A} \int_0^1 \sin^2 \pi r \, (w + 2\overline{w}) \, dr \Big\} \quad .$$

We write this as

$$\frac{B''(0)}{2} \frac{1}{\gamma} \frac{d\overline{c}_1}{d\tau} = \frac{B''(0)}{2} \overline{c}_1 + \frac{\lambda}{\gamma} |c_1|^2 \overline{c}_1 \ , \qquad (1.4.7)$$

where

$$\gamma = \frac{1 + \frac{A^2}{B_c} M_1^+}{1 - \frac{A^2}{B_c} (M_1^+)^2} \ ,$$

and $\frac{\lambda}{\gamma}$ is twice the quantity in braces in the previous equation.

To solve (1.4.7) we write $c_1(\tau) = c(\tau) \exp(-i\omega(\tau))$, substitute into (1.4.7), and equate real and imaginary parts to zero. The result is

$$\frac{B''(0)}{2} \frac{dc}{d\tau} = \frac{B''(0)}{2} (\mathrm{Re}\,\gamma) c + (\mathrm{Re}\,\lambda) \, c^3, \qquad (1.4.8)$$

$$\frac{B''(0)}{2} \frac{d\omega}{d\tau} = \frac{B''(0)}{2} (\mathrm{Im}\,\gamma) \, c + (\mathrm{Im}\,\gamma) \, c^3 \quad . \qquad (1.4.9)$$

Equation (1.4.8) is the same as (1.2.23) and has the solution

$$c(\tau) = \frac{c(\infty) \, c(0) \exp(\tau \, \mathrm{Re}\gamma)}{\left\{ (c(0))^2 (\exp(2\tau \, \mathrm{Re}\gamma) - 1) + (c(\infty))^2 \right\}^{\frac{1}{2}}}$$

where

$$c(\infty) = \left( - \frac{B''(0)}{2} \frac{\mathrm{Re}\gamma}{\mathrm{Re}\lambda} \right)^{\frac{1}{2}} \quad .$$

Then the solution to (1.4.9) is given by

$$\omega(\tau) = \omega(0) + \tau \operatorname{Im}\gamma + \frac{\operatorname{Im}\lambda}{B''(0)/2} \int_0^{\tau} c^2(s)\, ds .$$

As $\tau \to \infty$,

$$\omega(\tau) \sim \tau \left(\operatorname{Im}\gamma - \frac{\operatorname{Re}\gamma \operatorname{Im}\lambda}{\operatorname{Re}\lambda}\right) .$$

The asymptotic expansion of the solution to (1.1.1) and (1.1.2) in this case is therefore

$$X \sim A + 2\varepsilon\, c(\tau)\cos(at-\omega(\tau)) \sin\pi r$$
$$+ \varepsilon \operatorname{Re} \sum_{n=2}^{\infty} c_n^{\pm}(0) \exp \sigma_n^{\pm} t \sin n\pi r + O(\varepsilon^2) ,$$

$$Y \sim \frac{B_c}{A} + 2\varepsilon\, c(\tau) \cos(at-\omega(\tau))\, (M_1^+ + \overline{M_1^+}) \sin\pi r$$
$$+ \varepsilon \operatorname{Re} \sum_{n=2}^{\infty} c_n^{\pm}(0) \exp \sigma_n^{\pm} t\, M_n^{\pm} \sin n\pi r + O(\varepsilon^2) .$$

As $t \to \infty$ these solutions tend to the periodic solution

$$X \sim A + \sqrt{B-B_c}\; 2\sqrt{\frac{\operatorname{Re}\gamma}{\operatorname{Re}\lambda}} \cos\left\{t(a-(B-B_c)[\operatorname{Im} - \frac{\operatorname{Re}\gamma \operatorname{Im}\lambda}{\operatorname{Re}\lambda}])\right\}$$
$$\times \sin\pi r + O(B-B_c) , \qquad (1.4.10)$$

$$Y \sim \frac{B_c}{A} + \sqrt{B-B_c}\; 2\sqrt{-\frac{\operatorname{Re}\gamma}{\operatorname{Re}\lambda}} \cos\left\{t(a-(B-B_c)\right.$$
$$\left.\times \left[\operatorname{Im}\gamma - \frac{\operatorname{Re}\gamma \operatorname{Im}\lambda}{\operatorname{Re}\lambda}\right])\right\} (M_1^+ + \overline{M_1^+}) \sin \pi r$$
$$+ O(B-B_c) . \qquad (1.4.11)$$

It is seen that the amplitude of the disturbance is $O\left((B-B_c)^{\frac{1}{2}}\right)$ and the frequency shift is $O(B-B_c)$.

Once again, this expansion is valid only when $\sigma_1^{\pm}$ are the only eigenvalues which have positive real parts. This restriction would appear to be more important for the qualitative understanding of periodic solutions when $B-B_c$ is not small than the analogous restriction was for the bifurcation of steady states. There the shape of finite amplitude disturbances was essentially the same as the shape of infinitesimal disturbances. The periodic disturbances of this section, however, cannot possibly show travelling waves, since they are time-periodic multiples of the function $\sin\pi r$; that is, standing waves. Further, the neutral stability curve for the eigenfunctions corresponding to $\sigma_n^{\pm}$ in region III is $B_c = 1+A^2 + n^2\pi^2 D(1+\vartheta)$. For a small value of D, say $D = 10^{-3}$, many eigenfunctions will be excited even when $B-B_c$ is as small as 1. Each would oscillate with a different period, so that the resulting disturbance may be expected to be a complicated interaction of all of them. Consequently, an approach different from eigenfunction expansions is likely to be necessary to account for the other features of the oscillations exhibited by the model. The next section is the beginning of an attempt at such an approach.

## 1.5 Concentration Waves - Diffusion Absent

If diffusion is absent, the rate equations (1.1.1) and (1.1.2) become

$$\frac{\partial X}{\partial t} = A - (B + 1) X + X^2 Y \tag{1.5.1}$$

and

$$\frac{\partial Y}{\partial t} = BX - X^2 Y \; . \tag{1.5.2}$$

These are in effect a pair of coupled autonomous ordinary differential equations in the time; space does not enter, except through the initial conditions.

The unique critical point of (1.5.1) and (1.5.2) is $X = A$, $Y = B/A$. It is unstable if $B > 1 + A^2$. (If diffusion were included, the critical value of B for instability of the uniform solution would be $B = 1 + A^2 + \pi^2 D(1+\vartheta)$ if $\vartheta$ is sufficiently small, as was calculated in section 1.1.) If the critical point is unstable, it is found that phase trajectories starting near the critical point run onto a limit cycle, which can be denoted by $X_o(t)$, $Y_o(t)$. Since (1.5.1) and (1.5.2) are autonomous, the functions $X_o(t-\eta)$, $Y_o(t-\eta)$ also represent periodic solutions to (1.5.1) and (1.5.2), where $\eta$ is an arbitrary function of r.

Lavenda, Nicolis, and Herschkowitz-Kaufman [6] have studied the ordinary differential equations (1.5.1) and (1.5.2) numerically and analytically for the values $B = 77$, $A = 8 \cdot 2$. In this case the limit cycle is a relaxation oscillation, characterized by (nearly) discontinuous jumps. Solutions starting from initial conditions near the critical point run quickly onto the limit cycle.

Thus, after a short period of time, the solution of (1.5.1) and (1.5.2) may be considered to be of the form $X_o(t-\eta)$, $Y_o(t-\eta)$, where $\eta$ is determined from the initial conditions, and represents the time taken to reach the limit cycle from time $t = 0$. Since the initial conditions for the (degenerate) partial differential equations (1.5.1) and (1.5.2) depend on r, so does the phase shift $\eta(r)$. The functional form of the oscillation in space is therefore that of a travelling wave with wave speed $c(r) = \eta(r)/r$.

The rest of this section consists of calculations of the form and period of the relaxation oscillation for the choice $B >> 1$. The calculations done here are similar to those done for the van der Pol equation in Julian Cole's book [1]. They give a more accurate description than the phase plane arguments of Lavenda, Nicolis, and Herschkowitz-Kaufman. (The theory of Pontryagin [13] and Mishchenko [10], which examines discontinuous oscillations in detail using phase plane arguments, does not apply to (1.5.1) and (1.5.2) without modification.) It will be found that, in contrast to most singular perturbation calculations, the equations to be studied are not derived as the result of a limit process from (1.5.1) and (1.5.2).

It is possible to eliminate Y from (1.5.1) and (1.5.2) by solving (1.5.1) for Y in terms of X and $\frac{dX}{dt}$ (there will be no confusion in replacing $\frac{\partial}{\partial t}$ by $\frac{d}{dt}$), and then substituting the values of Y and $\frac{dY}{dt}$ into (1.5.2). The result is a second order equation for X which, however, contains a term $(\frac{dX}{dt})^2$. This may be removed by the transformation $X = \frac{A}{u}$. (The transformation $X = A/(1+A\xi)$, employed by Lefever and Nicolis [7], accomplishes the same thing.) The resulting differential equation for u is

$$\frac{d^2u}{dt^2} + \left\{\frac{A^2}{u^2} + 2u - \nu\right\} \frac{du}{dt} + A^2 \left\{1 - \frac{1}{u}\right\} = 0 \ , \qquad (1.5.3)$$

where $\nu = B+1 >> 1$. This equation is clearly equivalent to (1.5.1) and (1.5.2). We prefer to use (1.5.3) since it is of the form

$$u'' + f(u)u' + g(u) = 0 \ ,$$

and such equations have been intensively studied. The steady state for (1.5.3) is $u = 1$. The restoring force $g(u)$ is negative for $u < 1$ and positive for $u > 1$; it tends to $A^2$ as $u \to +\infty$ and to $-\infty$ as $u \to 0$. The damping $f(u)$ is negative for $u = 1$ but tends to $+\infty$ as $u \to \infty$ and as $u \to 0$. (We always work in the region $u > 0$ since it corresponds to positive concentrations of reactants.) Thus (1.5.3) represents a self-excited oscillation, and the existence of a limit cycle in the unstable case is guaranteed by a minor extension of the Levinson-Smith theorem [8], even when B is not large.

We now proceed to the calculation of the limit cycle in the case $B+1 = \nu >> 1$. The perturbation argument is that, in the presence of a small or large parameter, certain terms in the differential equation are negligible in the leading order. In singular perturbations, the negligible terms are different in different regions of the motion. In regions of slow time variation, or outer regions, the acceleration term $u''$ is negligible. In regions of fast time variation (inner regions or jumps), the restoring force is negligible. Transitional regions occur when representatives from all three terms in (1.5.3) are important. We may expect the solution to increase in amplitude when the damping is negative, and decrease when it is positive. Thus the approximate size of the limit cycle will be determined by the sign changes of the damping. It is seen from (1.5.3) that there are two distinct regimes: one where $u \sim \nu$, and one where $u \sim \nu^{-\frac{1}{2}}$. The following regions occur in the description of the motion: the upper outer region, where $u \sim \nu$ and time variations are slow; the upper transition region; the jump down; the lower outer region, where $u \sim \nu^{-\frac{1}{2}}$; the lower transition region; the jump up to the upper outer region. In each region a separate asymptotic expansion will be necessary. Since the jumps join regions of differing order of magnitude for u, we may expect a certain asymmetry in the equations for the jumps. It will be found that the equations contain the parameter $\nu$ explicitly, in contrast to the usual situation for singular perturbations. The balancing of the various terms will require that there be several natural time scales on which the motion progresses.

The upper outer solution

The asymptotic expansion in this region will be $u \sim \nu u_o + u_1 + \nu^{-1} u_2 + \ldots$. We want to balance the second two terms of (1.5.3), so the appropriate time scale is $\frac{d}{dt} \sim \nu^{-2}$. Let $\tau = \nu^{-2} t$. Substitution of the expansion into (1.5.3), and equation of coefficients of powers of $\nu$ to zero, yields the following hierarchy of equations:

$$(2u_o - 1)\frac{du_o}{d\tau} + A^2 = 0 \,, \tag{1.5.4}$$

$$(2u_o - 1)\frac{du_1}{d\tau} + 2\frac{du_o}{d\tau}u_1 - \frac{A^2}{u_o} = 0 \,, \tag{1.5.5}$$

$$(2u_o - 1)\frac{du_2}{d\tau} + 2\frac{du_o}{d\tau}u_2 + 2u_1\frac{du_1}{d\tau} + \frac{A^2 u_1}{u_o^2} = 0 \,. \tag{1.5.6}$$

The solution of (1.5.4) is found by separation of variables:

$$(2u_o - 1)\, du_o = -A^2 d\tau \ .$$

Thus

$$-(u_o - \tfrac{1}{2})^2 = A^2 \tau + C \ . \tag{1.5.7}$$

Equation (1.5.7) represents a family of coaxial parabolas with vertices at $u_o = \frac{1}{2}$. Since the differential equation is autonomous, we may choose the time origin wherever is convenient. If $C = 0$, then $u_o$ has its vertical tangent when $\tau = 0$. We choose the upper branch of the parabola since the solution is going to have to jump down to the lower outer region. Thus

$$u_o = \tfrac{1}{2} + A\sqrt{-\tau} \ . \tag{1.5.8}$$

Next, (1.5.5) may be written, using the chain rule and (1.5.4), as

$$\frac{du_1}{du_o} + \frac{2}{2u_o - 1} u_1 = -\frac{1}{u_o} \ ,$$

that is

$$\frac{1}{u_o - \frac{1}{2}} \frac{d}{du_o} \left[ (u_o - \tfrac{1}{2}) u_1 \right] = -\frac{1}{u_o} \ .$$

Therefore

$$u_1 = \frac{1}{u_o - \frac{1}{2}} \left( -u_o + \tfrac{1}{2} \log u_o + A_1 \right) ,$$

where $A_1$ is a constant of integration, to be determined from matching. Using (1.5.8) we obtain

$$u_1 = \frac{1}{A\sqrt{-\tau}} \left\{A_1 - \tfrac{1}{2}(1+\log 2) - A\sqrt{-\tau} + \tfrac{1}{2}\log(1+2A\sqrt{-\tau})\right\} \qquad (1.5.9)$$

As $\tau \to 0-$, $u_1$ has the expansion

$$u_1 \sim \frac{1}{A\sqrt{-\tau}} \left\{A_1 - \tfrac{1}{2}(1+\log 2)\right\} - A\sqrt{-\tau} - \frac{8}{3}\tau + O((-\tau)^{3/2}) . \quad (1.5.10)$$

The lower outer solution

In this region the asymptotic expansion will be $u \sim \nu^{-\frac{1}{2}} w_o + \nu^{-1} w_1 + \ldots$, and in order to balance the second two terms of (1.5.3) we let $\frac{d}{dt} \sim 1$. Then the hierarchy of equations is

$$\left(\frac{A^2}{w_o^2} - 1\right) \frac{dw_o}{dt} - \frac{A^2}{w_o} = 0 \ , \qquad (1.5.11)$$

$$\left(\frac{A^2}{w_o^2} - 1\right) \frac{dw_1}{dt} + w_1\left(\frac{A^2}{w_o^2} - \frac{2A^2}{w_o^3}\frac{dw_o}{dt}\right) + A^2 = 0 . \qquad (1.5.12)$$

The solution to (1.5.11) is

$$A^2 \log w_o - \tfrac{1}{2} w_o^2 = A^2 t + C .$$

Since the solution is going to have to jump up to the upper outer region, we choose the lower branch of this function; it has a vertical tangent at $w_o = A$. Call the time at which the tangent is vertical $t_j$ $(=t_j(\nu))$. Thus

$$A^2 \log w_o - A^2 \log A - \tfrac{1}{2} w_o^2 + \tfrac{1}{2}A^2 = A^2(t-t_j) .$$

Let $\hat{t} = t - t_j$; then the lower outer limit will have $\hat{t}$ fixed. Thus

$$A^2 \log w_o - A^2 \log A - \tfrac{1}{2} w_o^2 + \tfrac{1}{2}A^2 = A^2 \hat{t} \ . \qquad (1.5.13)$$

Next, (1.5.12) may be written

$$\frac{dw_1}{dw_o} + \left(\frac{1}{w_o} - \frac{2A^2}{w_o(A^2-w_o^2)}\right) w_o + 1 = 0 ,$$

or

$$\frac{d}{dw_o} \left(\frac{A^2-w_o^2}{w_o} w_1\right) = \frac{w_o^2-A^2}{w_o} .$$

Therefore

$$w_1 = \frac{1}{A^2-w_o^2} \left\{ \tfrac{1}{2}w_o^3 - A^2 w_o \log w_o + \mathcal{D}_1 w_o \right\} , \tag{1.5.14}$$

where $\mathcal{D}_1$ is a constant of integration.

We shall be interested in the expansions of $w_o$ and $w_1$ as $\hat{t} \to -t_j$ and as $\hat{t} \to 0-$. We postpone consideration of the first limit for a while, but can write immediately that as $\hat{t} \to 0-$,

$$w_o \sim A\,(1 - \sqrt{-\hat{t}} - \tfrac{1}{6}\hat{t} + \ldots) \tag{1.5.15}$$

and

$$w_1 \sim \frac{\tfrac{1}{2}A^2 - A^2 \log A + \mathcal{D}_1}{2A} \frac{1}{\sqrt{\hat{t}}} + \frac{1}{12} A - \frac{1}{6} A \log A + \frac{1}{6}\frac{\mathcal{D}_1}{A}$$
$$+ O(\sqrt{-\hat{t}}) . \tag{1.5.16}$$

<u>The inner solutions</u>

The appropriate time scale to balance the first two terms of (1.5.3) is $\frac{d}{dt} \sim \nu$. In the original variables, the leading equation for the jumps is thus (in both cases)

$$\frac{d^2u}{dt^2} + \left\{\frac{A^2}{u^2} + 2u-\nu\right\} \frac{du}{dt} = 0 \ , \qquad (1.5.17)$$

or

$$\frac{du}{dt} + u^2 - \nu u - \frac{A^2}{u} = C \ . \qquad (1.5.18)$$

Figure 1.5.1 shows the phase trajectories of equation (1.5.17). The line $u' = 0$ is singular. It is seen that there are two distinguished trajectories QR and ST which correspond to a jump up between two finite values of u, and to a jump down. Other trajectories start at $u = 0$, $u' = \infty$ or $u = \infty$, $u' = -\infty$ and are not of interest. The points Q and S are double zeroes of the cubic $u^2 - \nu u - A^2/u = C$, while R and T are simple zeroes. For the jump down it will be necessary that S match with the jump-off point $u = \frac{1}{2}\nu$ of the upper outer solution, at least to $o(1)$. This can be done by proper choice of C. For the jump up, Q must match with the jump-off point $u = A\nu^{-\frac{1}{2}}$. This can be done by another choice of C.

An important point is that in the jump down, when (at least at first) $u \sim \nu$, it is still necessary to include the term $\frac{A^2}{u^2}$ in equation (1.5.17). If it is omitted, the phase trajectories are no longer cubics but parabolas, and these have completely the wrong behavior for jumps. In the jump up, the term 2u must be included for the same reason. Although these terms are quantitatively negligible at the beginning of the jumps, they are important at the end. Thus it will be necessary to treat them as being of honorary order $\nu$. The asymmetry introduced is not found in the similar equations for the van der Pol oscillator. In this case, the inclusion of the extra

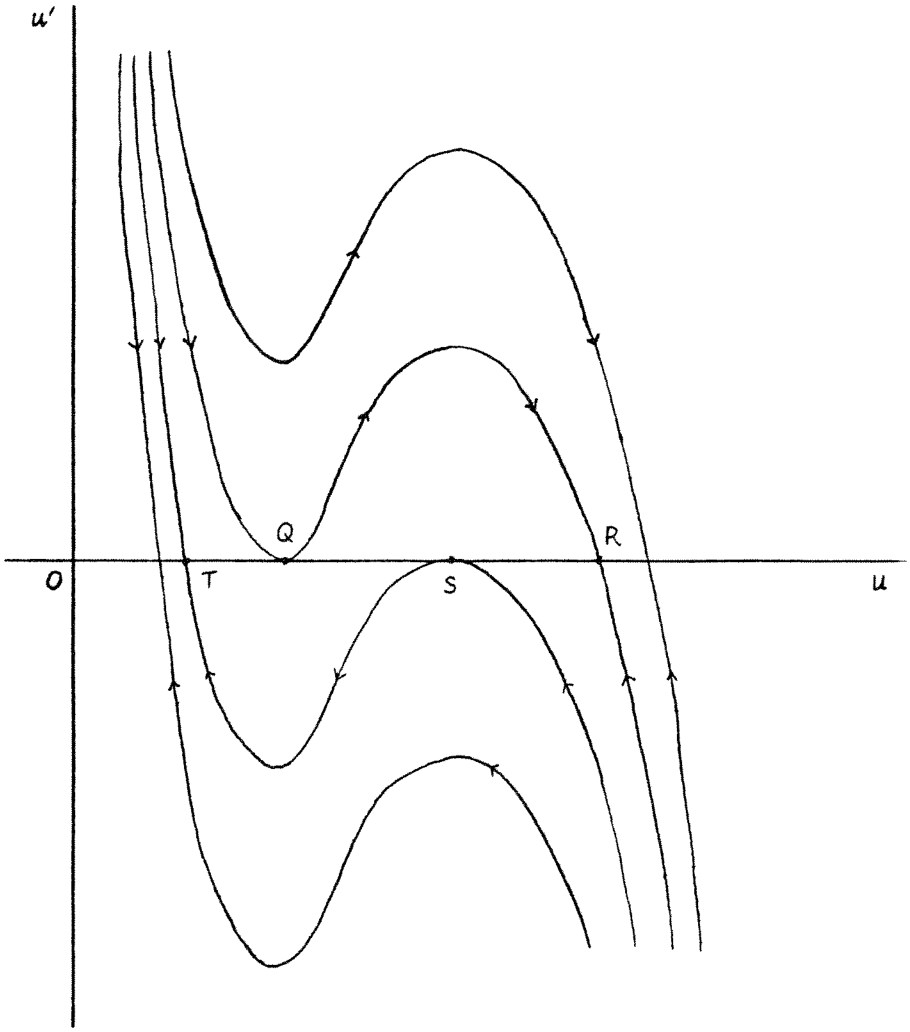


Figure 1.5.1. Phase trajectories of equation (1.5.17).

terms implies that the inner equations are not obtained as the result of a limit process, and the equations in the hierarchy all contain $\nu$ explicitly.

For the jump down we try $u \sim \nu\, g_o(\nu,\bar{t}) + \beta_1(\nu)\, g_1(\nu,\bar{t}) + \beta_2(\nu) g_2(\nu,\bar{t}) + \ldots$, where $\bar{t} = \nu(t-\delta(\nu))$. There is a possible time shift, because only $\frac{d\bar{t}}{dt}$ is determined from balancing considerations. The coefficients $\beta_1(\nu)$, $\beta_2(\nu), \ldots$, and $\delta(\nu)$ are to be found from matching. Since we treat $A^2/u^2$ as being of honorary order $\nu$, the hierarchy of equations obtained from (1.5.3) is

$$\frac{d^2 g_o}{d\bar{t}^2} + \left[\frac{A^2}{\nu^3 g_o^2} + 2g_o - 1\right] \frac{dg_o}{d\bar{t}} = 0\,, \tag{1.5.19}$$

$$\frac{d^2 g_1}{d\bar{t}^2} + \left[\frac{A^2}{\nu^3 g_o^2} + 2g_o - 1\right] \frac{dg_1}{d\bar{t}} + \left[2 - \frac{2A^2}{\nu^3 g_o^3}\right]\frac{dg_o}{d\bar{t}}\, g_1 = 0. \tag{1.5.20}$$

Integrating (1.5.19) once, we have

$$\frac{dg_o}{d\bar{t}} + \left[-\frac{A^2}{\nu^3 g_o} + g_o^2 - g_o\right] = C_o\,. \tag{1.5.21}$$

As $\bar{t} \to -\infty$, we want $g_o$ to tend to $a = \frac{1}{2} + o(1)$ and $\frac{dg_o}{d\bar{t}}$ to tend to zero; $a$ must be a double root of $-\frac{A^2}{\nu^3 g_o} + g_o^2 - g_o = C_o$. Call the other root $\beta$; then (1.5.21) becomes

$$\frac{dg_o}{d\bar{t}} = -\frac{(g_o-a)^2(g_o-\beta)}{\beta} = (a-g_o)^2\left(\frac{\beta}{g_o} - 1\right)\,. \tag{1.5.22}$$

The condition that $a$ be a double root requires that

$$2a^3 - a^2 + \frac{A^2}{\nu^3} = 0\,.$$

Three iterations using Newton's method on this equation yield

$$\alpha = \tfrac{1}{2}\left(1 - \frac{4A^2}{\nu^3} + \frac{32A^4}{\nu^6} + O(\nu^{-9})\right) \qquad (1.5.23)$$

and

$$\beta \equiv 1 - 2\alpha = \frac{4A^2}{\nu^3}\left(1 - \frac{8A^2}{\nu^3} + O(\nu^{-6})\right). \qquad (1.5.24)$$

From equation (1.5.22) we see that the decay of $g_o$ to $\alpha$ as $\bar{t} \to -\infty$ is only algebraic, whereas the decay to $\beta$ as $\bar{t} \to +\infty$ is exponential. As $\bar{t} \to -\infty$, $g_o$ has the expansion

$$g_o = \alpha + \frac{A_1}{\bar{t}}\; A_{1,2}\; \frac{\log(-\bar{t})}{\bar{t}^2} + \frac{A_2}{\bar{t}^2} + A_{2,3}\frac{\log^2(-\bar{t})}{\bar{t}^3} + \ldots, \qquad (1.5.25)$$

where

$$A_1 = (1 - \tfrac{\beta}{\alpha})^{-1} = 1 + \frac{8A^2}{\nu^3} + \ldots ,$$

$$A_{1,2} = -\frac{\beta}{\alpha^2}(1 - \tfrac{\beta}{\alpha})^{-3} = -\frac{16A^2}{\nu^3}\left(1 - \frac{24A^2}{\nu^3} + \ldots\right),$$

$$A_2 = \tfrac{1}{2}A_{1,2}\,.$$

As $\bar{t} \to +\infty$, $g_o$ has the expansion

$$g_o = \beta + O\left(\exp(-\frac{(\beta-\alpha)^2}{\beta}\,\bar{t})\right) \qquad (1.5.26)$$

$$= \frac{4A^2}{\nu^3}(1 - \frac{8A^2}{\nu^3} + \ldots) + \text{transcendentally small terms.}$$

Next, (1.5.20) implies

$$\frac{d}{d\bar{t}}\left\{\frac{dg_1}{d\bar{t}} + g_1\left(\frac{A^2}{\nu^3 g_o^2} + 2g_o - 1\right)\right\} = 0\,.$$

Certainly $g_1 = h_1 \dfrac{dg_1}{d\bar{t}}$, where $h_1$ is a constant of integration, is a solution. The general solution will be the sum of this and the particular integral of

$$\frac{dg_1}{d\bar{t}} + \left(\frac{A^2}{\nu^3 g_o^2} + 2g_o - 1\right) = k_1 . \tag{1.5.27}$$

We can find the leading order contribution to $g_1$ as $\bar{t} \to \pm\infty$. As $\bar{t} \to -\infty$, equation (1.5.27) is asymptotic to

$$\frac{dg_1}{d\bar{t}} + \left\{\frac{1}{\bar{t}}(2+\dots) + \frac{\log(-\bar{t})}{\bar{t}^2}\left(-32\frac{A^2}{\nu^3}+\dots\right) + \frac{1}{\bar{t}^2}\left(\frac{32A^2}{\nu^3}+\dots\right)\right\} g_1 = k_1 .$$

Thus the particular integral is asymptotic to

$$g_{1p} = k_1\left\{\left(\frac{1}{3} + O(\nu^{-6})\right)\bar{t} + \left(\frac{16}{3}\frac{A^2}{\nu^3}+\dots\right)\log(-\bar{t}) + \frac{8A^2}{\nu^3} + \dots + O\left(\frac{\log(-\bar{t})}{\bar{t}}\right)\right\},$$

and hence as $\bar{t} \to -\infty$,

$$g_1 \sim \frac{1}{3}k_1\bar{t} + \dots .$$

The homogeneous solution does not enter until later in the expansion. As yet the constant $k_1$ is not known. As $\bar{t} \to +\infty$, (1.5.27) is asymptotic to

$$\frac{dg_1}{d\bar{t}} + \left(\frac{A^2}{\nu^3\beta^2} + 2\beta - 1 + \text{TST}\right) g_1 = k_1 .$$

Thus as $\bar{t} \to +\infty$, $g_1 = \dfrac{16A^2}{\nu^3} k_1 + \text{TST}$.

The expansion for the jump up will be $u \sim \nu^{-\frac{1}{2}} z_o + \mu_1(\nu) z_1 + \dots$, with the time $\tilde{t} = \nu(\hat{t} - \chi(\nu))$. As was mentioned above, it will be necessary to treat the term 2u as being of order $\nu$. The hierarchy of equations that results is

$$\frac{d^2 z_o}{d\tilde{t}^2} + \left[\frac{A^2}{z_o^2} + \frac{2z_o}{\nu^{3/2}} - 1\right]\frac{dz_o}{d\tilde{t}} = 0 \,, \tag{1.5.28}$$

$$\frac{d^2 z_1}{d\tilde{t}^2} + \left[\frac{A^2}{z_o^2} + \frac{2z_o}{\nu^{3/2}} - 1\right]\frac{dz_1}{d\tilde{t}} + \frac{dz_o}{d\tilde{t}}\left[\frac{2}{\nu^{3/2}} - \frac{2A^2}{z_o^3}\right]z_1 = 0 \,. \tag{1.5.29}$$

One integration of (1.5.28) yields

$$\frac{dz_o}{d\tilde{t}} + \left[-\frac{A^2}{z_o} + \frac{z_o^2}{\nu^{3/2}} - z_o\right] = \mathcal{C} \,. \tag{1.5.30}$$

As $\tilde{t} \to -\infty$ we want $z_o = A + o(1)$ and $\frac{dz_o}{d\tilde{t}} \to 0$; the value $\phi$ that $z_o$ attains must be a double root of

$$-\frac{A^2}{z_o} + \frac{z_o^2}{\nu^{3/2}} - z_o = \mathcal{C} \,.$$

If the other root is called $\psi$, then (1.5.30) becomes

$$\frac{dz_o}{d\tilde{t}} = \frac{1}{\nu^{3/2}} \frac{(z_o - \phi)^2(\psi - z_o)}{z_o} \,, \tag{1.5.31}$$

and $\phi$ must satisfy the equation $2\phi^3 - \nu^{3/2}\phi^2 + \nu^{3/2}A^2 = 0$. Three iterations using Newton's method yield

$$\phi = A\left(1 + \frac{A^2}{\nu^{3/2}} + \frac{5}{2}\frac{A^2}{\nu^2} + O(\nu^{-9/2})\right) ,$$

$$\psi \equiv \nu^{3/2} - 2\phi = \nu^{3/2}\left(1 - \frac{2A}{\nu^{3/2}} - \frac{2A^2}{\nu^3} - \frac{5A^3}{\nu^{9/2}} + O(\nu^{-6})\right).$$

From (1.5.31) it is found that as $\tilde{t} \to -\infty$,

$$z_o = \phi + \frac{\mathcal{g}_1}{\tilde{t}} + \mathcal{g}_{1,2}\frac{\log(-\tilde{t})}{\tilde{t}^2} + \frac{\mathcal{g}_2}{\tilde{t}^2} + \ldots , \tag{1.5.32}$$

where

$$\mathcal{g}_1 = -\nu^{3/2}\left(\frac{\psi}{\phi} - 1\right)^{-1} = -A\left(1 + \frac{4A}{\nu^{3/2}} + \ldots\right),$$

$$\mathcal{g}_{1,2} = \nu^3 \frac{\psi}{\phi^2}\left(\frac{\psi}{\phi} - 1\right)^{-3} = A\left(1 + \frac{8A}{\nu^{3/2}} + \ldots\right),$$

$$\mathcal{g}_2 = \tfrac{1}{2}\mathcal{g}_{1,2} .$$

As $\tilde{t} \to \infty$,

$$z_o = \psi + \text{TST} = \nu^{3/2}\left(1 - \frac{2A}{\nu^{3/2}} - \frac{2A^2}{\nu^3} + \ldots\right) + \text{TST} . \tag{1.5.33}$$

Next, (1.5.29) implies

$$\frac{dz_1}{d\tilde{t}} + \left(\frac{A^2}{z_o^2} + \frac{2z_o}{\nu^{3/2}} - 1\right) z_1 = \mathcal{B}_1 , \tag{1.5.34}$$

where $\mathcal{B}_1$ is a constant of integration. As $\tilde{t} \to -\infty$, we find by the same method as for the jump down,

$$z_1 = \mathcal{B}_1\Big[\tfrac{1}{3}(1+O(\nu^{-3}))\,\tilde{t} + \tfrac{2}{3}\left(1 + \frac{4A}{\nu^{3/2}} + \ldots\right)\log(-\tilde{t})$$

$$- \tfrac{1}{2}\left(1 + \frac{4A}{\nu^{3/2}}\right)\Big] + O\left(\frac{\log(-\tilde{t})}{\tilde{t}^2}\right) . \tag{1.5.35}$$

As $\tilde{t} \to +\infty$,

$$z_1 = \frac{\mathcal{B}_1}{\dfrac{A^2}{\psi^2} + \dfrac{2\psi}{\nu^{3/2}} - 1} + \text{TST} = \mathcal{B}_1\left(1 + \frac{4A}{\nu^{3/2}} + \frac{19A^2}{\nu^3} + \ldots\right) + \text{TST}. \tag{1.5.36}$$

Leading order calculation of the period

Knowledge of the ends of the jumps enables us to make a first approximation to the period at this stage. The jumps themselves are treated as being instantaneous, and the period is the sum of the time taken for the upper outer solution to get from $u = \nu^{-\frac{1}{2}}\psi$ to $u = \frac{1}{2}\nu$ and the time taken for the lower outer solution to get from $u = \nu\beta$ to $u = \nu^{-\frac{1}{2}}A$. Substitution of these values into (1.5.8) and (1.5.13) yields

$$T = \frac{\nu^2}{4A^2}\left(1 - \frac{8A}{\nu^{3/2}} + \ldots\right) + \frac{3}{2}\log\nu - \log A - 2\log 2 + \ldots .$$

This formula agrees to leading order with the one calculated by phase plane methods by Lavenda, Nicolis, and Herschkowitz-Kaufman [6]. The form of the solution u(t) is shown in figure 1.5.2, and the concentration $X = \frac{A}{u}$ is shown in figure 1.5.3.

Although the inner and outer solutions match to leading order, the algebraic decay of the inner solutions as $\bar{t} \to -\infty$ and as $\tilde{t} \to -\infty$ means that higher order matching cannot be carried out. A more detailed computation of the solution, and thus of the period, requires the introduction of transition expansions. The upper transition solution must match the upper outer solution as $\tau \to 0-$ and the jump down as $\bar{t} \to -\infty$. The lower transition solution must match the lower outer solution as $\hat{t} \to 0-$ and the jump up as $\tilde{t} \to -\infty$. (Since the decay of the inner solutions is exponential as $\tilde{t} \to +\infty$ and $\bar{t} \to +\infty$, there is no trouble in matching them to the outer solutions there.) Each transition solution must contain representatives from all three terms in equation (1.5.3).

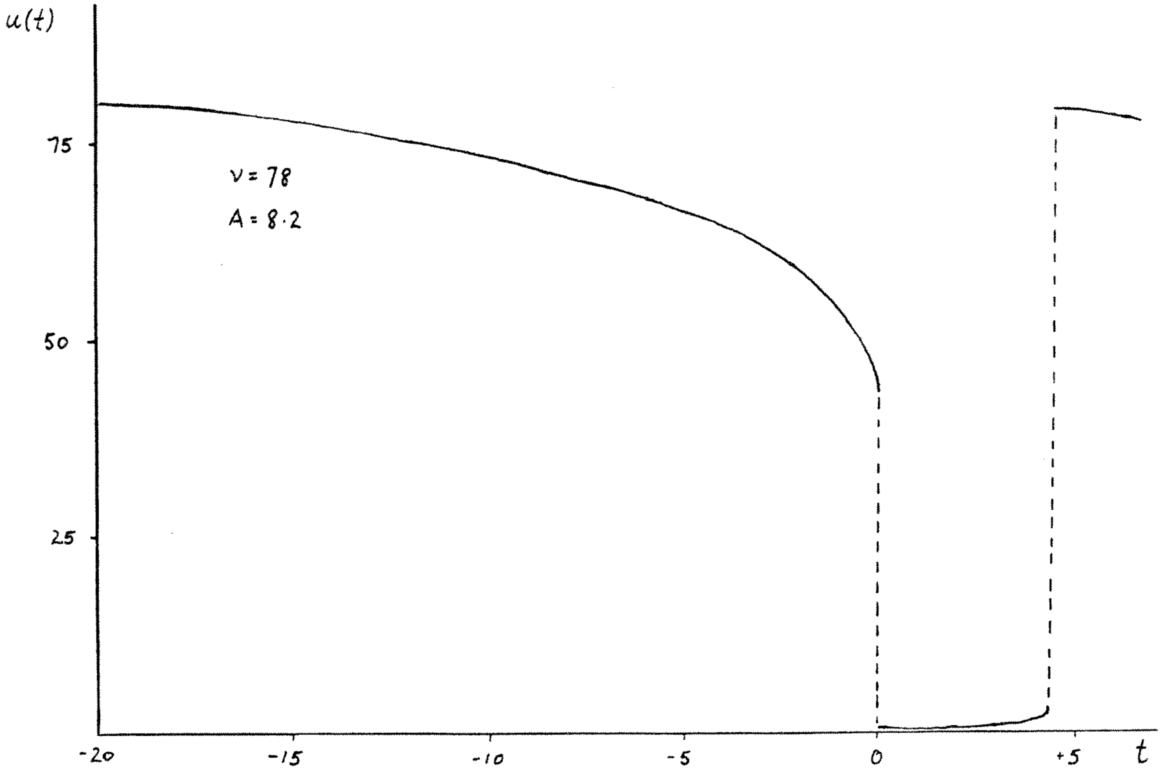


Figure 1.5.2. One oscillation of u(t).

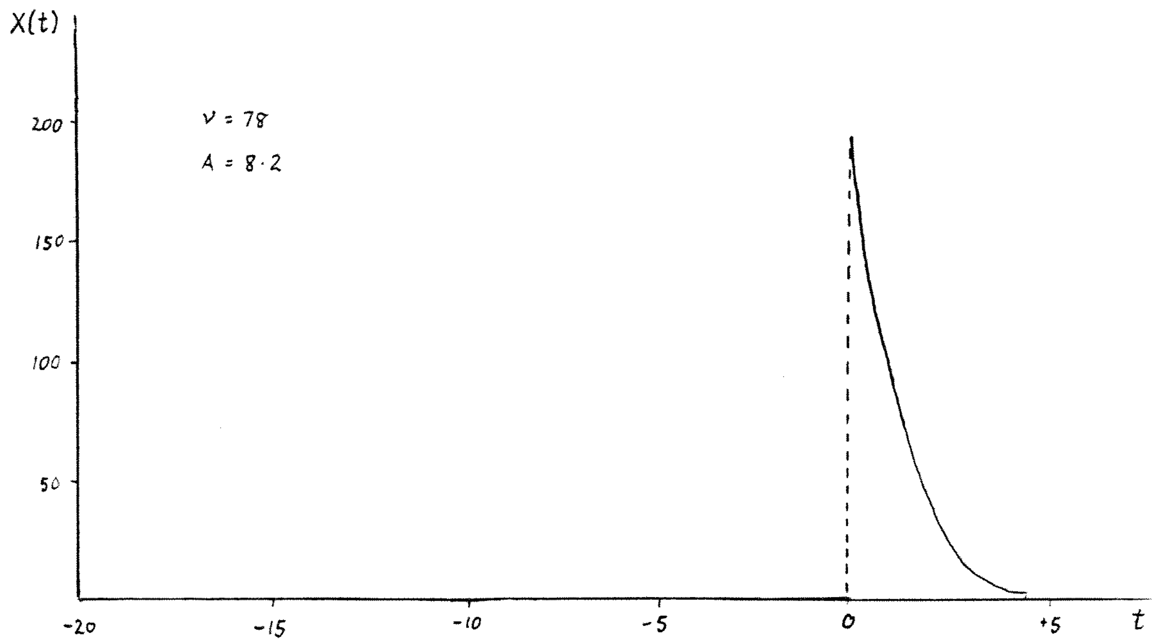


Figure 1.5.3. One oscillation of X = A/u. The concentration of X is nearly zero throughout most of the oscillation.

The upper transition solution

The necessary time scaling in this region is $\frac{d}{dt} \sim 1$, say $t^* = t-\rho(\nu)$, and the expansion is of the form $u \sim \frac{1}{2}\nu + f_1 + \nu^{-1} f_2 + \ldots$ . The hierarchy of equations is

$$\frac{d^2 f_1}{dt^{*2}} + 2f_1 \frac{df_1}{dt^*} + A^2 = 0 , \qquad (1.5.37)$$

$$\frac{d^2 f_2}{dt^{*2}} + 2f_1 \frac{df_2}{dt^*} + 2 \frac{df_1}{dt^*} f_2 - 2A^2 = 0 . \qquad (1.5.38)$$

One integration of (1.5.37) yields

$$\frac{df_1}{dt^*} + f_1^2 + A^2 t^* = 0 , \qquad (1.5.39)$$

where the constant of integration has been absorbed into $\rho(\nu)$. If we let $f_1 = V'/V = \frac{d}{dt^*} \log V$, then (1.5.39) becomes

$$\frac{d^2 V}{dt^{*2}} + A^2 t^* V = 0 . \qquad (1.5.40)$$

Substituting $z = \theta t^*$, where $\theta^2 = A^2/\theta$, we find that (1.5.40) becomes

$$\frac{d^2 V}{dz^2} + zV = 0 ,$$

which is Airy's equation for negative argument and has the solution

$$V = M\sqrt{-z}\;\; K_{\frac{1}{3}}\left(\tfrac{2}{3}(-z)^{3/2}\right) + N\sqrt{-z}\;\; I_{\frac{1}{3}}\left(\tfrac{2}{3}(-z)^{3/2}\right) .$$

$I_{\frac{1}{3}}$ and $K_{\frac{1}{3}}$ are modified Bessel functions. As $t^* \to -\infty$ (i.e., $z \to -\infty$) they have the expansions

$$K_{\frac{1}{3}}(\tfrac{2}{3}(-z)^{3/2}) = \tfrac{1}{2}\sqrt{3\pi}\ (-z)^{-\frac{3}{4}} \exp\left[-\tfrac{2}{3}(-z)^{3/2}\right]\left\{1-\frac{5}{48}(-z)^{-3/2}+\ldots\right\},$$

$$I_{\frac{1}{3}}(\tfrac{2}{3}(-z)^{3/2}) = \tfrac{1}{2}\sqrt{\frac{3}{\pi}}\ (-z)^{-\frac{3}{4}} \exp\left[\tfrac{2}{3}(-z)^{3/2}\right]\left\{1+\frac{5}{48}(-z)^{3/2}+\ldots\right\}. \tag{1.5.41}$$

In order to match to the upper outer solution, we need to choose the solution of (1.5.39) that behaves as $+\sqrt{-t^*}$ as $\tau \to 0-$. This can happen only if $N = 0$. This choice uses up one of the constants of integration; the other is in $\rho(\nu)$. Since $f_1 = V'/V$, we can choose $M = 1$ and obtain

$$V(z) = \begin{cases} \sqrt{-z}\ K_{\frac{1}{3}}(\tfrac{2}{3}(-z)^{3/2}) & \text{for } z < 0 \\ \\ \dfrac{\pi}{\sqrt{3}}\ \sqrt{z}\ \left\{J_{\frac{1}{3}}(\tfrac{2}{3}z^{3/2}) + J_{-\frac{1}{3}}(\tfrac{2}{3}z^{3/2})\right\} & \text{for } z > 0\,. \end{cases} \tag{1.5.42}$$

As $t^* \to -\infty$, $f_1$ therefore has the expansion

$$f_1 = A\sqrt{-t^*} - \frac{1}{4t^*} - \frac{5}{32A}(-t^*)^{-5/2} + O((-t^*)^{-7/2})\,, \tag{1.5.43}$$

found from (1.5.41) and (1.5.42). To match to the jump down we take the limit $z \to \omega_o$, where $\omega_o$ is the first zero of the Airy function. It is a simple zero with the approximate value $\omega_o = 2.338$. As z tends to $\omega_o$,

$$V(z) \propto -(z-\omega_o) + \frac{1}{6}\omega_o(z-\omega_o)^3 + O((z-\omega_o)^5)\,. \tag{1.5.44}$$

As z tends to $\omega_o$, $t^* = A^{-\frac{2}{3}} z$ tends to $\theta_o = A^{-\frac{2}{3}}\omega_o$. So as $t^* \to \theta_o$,

$$f_1 = \frac{1}{t^*-\theta_o} - \tfrac{1}{3}A^{4/3}\omega_o(t^*-\theta_o) + O((t^*-\theta_o)^3)\,. \tag{1.5.45}$$

Next, (1.5.38) becomes upon integration

$$\frac{df_2}{dt^*} + 2f_1 f_2 = 2A^2 t^* + C_2 ,$$

that is

$$V^2 f_2 = \int_{-\infty}^{t^*} 2A^2 \lambda V^2(\lambda) d\lambda + \int_{-\infty}^{t^*} C_2 V^2(\lambda) d\lambda + D_2 .$$

In order to prevent exponential growth of $f_2$ as $t^* \to -\infty$, we must choose $D_2 = 0$. Thus

$$f_2(t^*) = \frac{C_2}{V^2} \int_{-\infty}^{t^*} V^2(\lambda) d\lambda + \frac{2A^2}{V^2} \int_{-\infty}^{t^*} \lambda V^2(\lambda) d\lambda . \qquad (1.5.46)$$

Using (1.5.41) and integrating by parts, we find that as $t^* \to -\infty$,

$$f_2 = -A\sqrt{-t^*} + \frac{C_2}{2A} \left\{ \frac{1}{\sqrt{-t^*}} + \frac{11}{12A} t^{*-2} \right\} + O((-t^*)^{-5/2}) . \quad (1.5.47)$$

Using (1.5.45) we find that as $t^* \to \theta_o$,

$$f_2 = \frac{1}{(t^* - \theta_o)^2} A^{-4/3} \left\{ C_2 \int_{-\infty}^{\theta_o} V^2(\lambda) d\lambda + 2A^2 \int_{-\infty}^{\theta_o} \lambda V^2(\lambda) d\lambda \right\} \left\{ 1 + \tfrac{1}{3} A^{4/3} \omega_o (t^* - \theta_o)^2 + \ldots \right\} . \qquad (1.5.48)$$

<u>The lower transition solution</u>

In this region it is necessary to use the expansion $u \sim \nu^{-\frac{1}{2}} A + \nu^{-5/6} y_1 + \nu^{-7/6} y_2 + \ldots$ and to take $\frac{d}{dt} \sim \nu^{\frac{2}{3}}$, so that $t^+ = \nu^{2/3}(\hat{t} - \lambda(\nu))$. The hierarchy of equations is

$$\frac{d^2 y_1}{dt^{+2}} - \frac{2}{A} y_1 \frac{dy_1}{dt^+} - A = 0 , \qquad (1.5.49)$$

$$\frac{d^2y_2}{dt^{+2}} + \left[-\frac{2}{A}y_2 + \frac{3y_1^2}{A^2}\right]\frac{dy_1}{dt^+} - \frac{2}{A}y_1\frac{dy_2}{dt^+} - y_1 = 0 . \qquad (1.5.50)$$

One integration of (1.5.9) yields

$$\frac{dy_1}{dt^+} - \frac{1}{A}y_1^2 - At^+ = 0 , \qquad (1.5.51)$$

where once again the constant of integration has been absorbed into $\lambda(\nu)$. If we let $y_1 = -AV'/V$, then (1.5.51) becomes

$$\frac{d^2V}{dt^{+2}} + t^+V = 0 .$$

Thus

$$V(t^+) = M\sqrt{-t^+}\; K_{\frac{1}{3}}\left(\tfrac{2}{3}(-t^+)^{3/2}\right) + N\sqrt{-t^+}\; I_{\frac{1}{3}}\left(\tfrac{2}{3}(-t^+)^{3/2}\right) .$$

We want the solution of (1.5.51) that behaves as $-\sqrt{-\hat{t}}$ as $\hat{t} \to 0-$. This forces $N = 0$, and as before we may also choose $M = 1$. Thus

$$V(t^+) = \begin{cases} \sqrt{-t^+}\; K_{\frac{1}{3}}\left(\tfrac{2}{3}(-t^+)^{3/2}\right) & \text{if } t^+ < 0 \\ \frac{\pi}{\sqrt{3}}\sqrt{t^+}\left\{J_{\frac{1}{3}}\left(\tfrac{2}{3}t^{+3/2}\right) + J_{-\frac{1}{3}}\left(\tfrac{2}{3}t^{+3/2}\right)\right\} & \text{if } t^+ > 0 . \end{cases}$$

As $t^+ \to -\infty$, $y_1$ has the expansion

$$y_1 = -A\sqrt{-t^+} + \frac{A}{4t^+} + \frac{5A}{32}(-t^+)^{-5/2} + O(1-t^+)^{-7/2}) , \qquad (1.5.52)$$

and as $t^+ \to \omega_o$, $y_1$ has the expansion

$$y_1 = -A\left[\frac{1}{t^+-\omega_o} - \tfrac{1}{3}\omega_o(t^+-\omega_o) + O((t^+-\omega_o)^2)\right] . \qquad (1.5.53)$$

Next, one integration of (1.5.50) yields

$$\frac{dy_2}{dt^+} + 2\left(\frac{d}{dt^+}\log V\right) y_2 + \frac{y_1^3}{A^2} = -A \log V + \mathcal{E}_2 ,$$

or

$$\frac{1}{V^2}\frac{d}{dt^+}(V^2 y_2) - \frac{AV'^3}{V^3} = -A\log V + \mathcal{E}_2 . \tag{1.5.54}$$

A further integration together with the use of (1.5.51) and integration by parts gives

$$y_2 = \frac{\mathcal{F}_2}{V^2} + \frac{dy_1}{dt^+}\left(\frac{\mathcal{E}_2}{A} + \log V\right) - \frac{2A}{V^2}\int_{-\infty}^{t^+} V^2 \log V \, d\lambda + \tfrac{1}{2}\frac{y_1^2}{A} . \tag{1.5.55}$$

To prevent exponential growth of $y_2$ as $t^+ \to -\infty$, it is necessary to choose $\mathcal{F}_2 = 0$. As $t^+ \to -\infty$, $y_2$ then has the expansion

$$y_2 = A\left\{\frac{1}{6}t^+ + \frac{1}{8}\frac{\log(-t^+)}{\sqrt{-t^+}} + \left[\frac{1}{2}\frac{\mathcal{E}_2}{A} - \frac{1}{2}\log\sqrt{\frac{3\pi}{2}} + \frac{4}{9}\right]\frac{1}{\sqrt{-t^+}} + \dots\right\} , \tag{1.5.56}$$

and as $t^+ \to \omega_o$, $y_2$ has the expansion

$$y_2 = A\frac{\log(\omega_o - t^+)}{(t^+ - \omega_o)^2} + \frac{1}{(t^+ - \omega_o)^2}\left\{\mathcal{E}_2 - 2A\int_{-\infty}^{\omega_o} V^2 \log V d\lambda + \tfrac{1}{2}A + \dots\right\} . \tag{1.5.57}$$

Matching of the various expansions

Since the expressions for the functions to be matched and their expansions in the various time limits are complicated, we find it safer to go explicitly through the intermediate limit procedure in every case.

To match the upper outer and transition solutions, we consider the limit $\tau \to 0-$, $t^* \to -\infty$. We let $t_\eta = \frac{t-\rho(\nu)}{\eta(\nu)} < 0$ be fixed, where $1 \ll \eta \ll \nu^2$ as $\nu \to \infty$. Thus $t^* = \eta t_\eta$, $\tau = \nu^{-2}(\eta t_\eta + \rho)$. It may be assumed that $\rho \ll \eta$. From (1.5.8) and (1.5.10), the expansion of the upper outer solution in the intermediate variables is

$$u = \frac{\nu}{2} + A\sqrt{-\eta t_\eta - \rho} + \frac{\nu}{A\sqrt{-\eta t_{\eta} - \rho}} \left\{A_1 - \tfrac{1}{2}(1+\log 2)\right\}$$
$$- \frac{A}{\nu}\sqrt{-\eta t_\eta - \rho} + \ldots$$
$$= \frac{\nu}{2} + A\sqrt{-\eta t_\eta} - \frac{1}{2}\frac{A\rho}{\sqrt{-\eta t_\eta}} + \nu\,\frac{A_1 - \frac{1}{2}(1+\log 2)}{A}\,\frac{1}{\sqrt{-\eta t_\eta}}$$
$$- \frac{A}{\nu}\sqrt{-\eta t_\eta} + \ldots \quad . \tag{1.5.58}$$

From (1.5.43) and (1.5.47), the expansion of the upper transition solution in the intermediate variables is

$$u = \frac{\nu}{2} + A\sqrt{-\eta t_\eta} - \frac{A}{\nu}\sqrt{-\eta t_\eta} + \ldots \quad . \tag{1.5.59}$$

Both $\rho$ and $A_1$ should be determined from a comparison of (1.5.58) and (1.5.59). Thus we must choose $\rho = 0$ and $A_1 = \frac{1}{2}(1+\log 2)$. The terms omitted vanish faster than those matched.

To match the upper transition solution and the jump down, we take the limit $t^* \to \theta_0$, $\bar{t} \to -\infty$. We let $\nu^{-1} \ll \eta \ll 1$ and $t_\eta < 0$ be fixed. Then $\bar{t} = \nu(t-\delta(\nu)) = \nu(t^*-\delta(\nu)) = \nu\eta t_\eta$. Thus $t^* = \eta t_\eta + \delta$ and $t^* - \theta_0 = \eta t_\eta + \sigma(\nu)$ where $\sigma(\nu) = \delta(\nu) - \theta_0$. We may assume $\sigma \gg \eta$. In the intermediate variables the upper transition solution is

$$u = \frac{\nu}{2} + \frac{1}{\eta t_\eta + \sigma} - \tfrac{1}{3}A^{4/3}\omega_o(\eta t_\eta + \sigma) + \ldots$$

$$+ \frac{1}{\nu(\eta t_\eta + \sigma)^2} A^{-4/3}\left\{C_2 \int_{-\infty}^{\theta_o} V^2 d\lambda + 2A^2 \int_{-\infty}^{\theta_o} \lambda V^2 d\lambda\right\}$$

$$= \frac{\nu}{2} + \frac{1}{\eta t_\eta} - \frac{\sigma}{(\eta t_\eta)^2} + \ldots - \tfrac{1}{3}A^{4/3}\omega_o \eta t_\eta + \ldots$$

$$+ \frac{1}{\eta(\eta t_\eta)^2} A^{-4/3}\left\{C_2 \int_{-\infty}^{\theta_o} V^2 d\lambda + 2A^2 \int_{-\infty}^{\theta_o} \lambda V^2 d\lambda\right\},$$

(1.5.60)

and the inner solution is

$$u = \frac{\nu}{2}\left(1 - \frac{4A^2}{\nu^3} + \ldots\right) + \left(1 + \frac{8A^2}{\nu^3} + \ldots\right)\frac{1}{\eta t_\eta} + \ldots$$

$$+ \beta_1(\nu)\tfrac{1}{3}k_1 \nu \eta t_\eta + \ldots \quad . \qquad (1.5.61)$$

Comparison of (1.5.60) and (1.5.61) shows that we must take $\beta_1 = \nu^{-1}$, $k_1 = -A^{4/3}\omega_o$, $\sigma = 0$, and $C_2 = -2A^2 \int_{-\infty}^{\theta_o} \lambda V^2 d\lambda \Big/ \int_{-\infty}^{\theta_o} V^2 d\lambda$. Thus the inner expansion is $u \sim \nu g_o + \nu^{-1} g_1 + \ldots$, and as $\bar{t} \to +\infty$,

$$u = \frac{4A^2}{\nu^3}\left(1 - \frac{8A^2}{\nu^3} + \ldots\right) - \frac{16A^2}{\nu^4} A^{4/3}\omega_o + \text{TST} . \qquad (1.5.62)$$

The time shift $\delta(\nu)$ is equal to $\theta_o = A^{-\frac{2}{3}}\omega_o$.

The limit to be taken in matching the lower outer and transition solutions is $\hat{t} \to 0-$, $t^+ \to -\infty$. We introduce $\eta(\nu)$ where $\nu^{-\frac{2}{3}} \ll \eta \ll 1$, let $t_\eta < 0$ be fixed, and put $t^+ = \nu^{\frac{2}{3}}(\hat{t} - \lambda(\nu)) = \nu^{\frac{2}{3}}\eta t_\eta$. Then $\hat{t} = \eta t_\eta + \lambda$. In the intermediate variables the outer expansion is

$$u = \frac{A}{\sqrt{\nu}}\left(1 - \sqrt{-\eta t_\eta - \lambda} - \frac{1}{6}(\eta t_\eta + \lambda) + \dots\right)$$

$$+ \frac{1}{\nu}\left[\frac{\frac{1}{2}A^2 - A^2 \log A + \mathcal{D}_1}{2A} \frac{1}{\sqrt{-\eta t_\eta - \lambda}}\right.$$

$$\left. + \frac{1}{12} A - \frac{1}{6} A \log A + \frac{1}{6} \frac{\mathcal{D}_1}{A} + \dots\right]$$

$$= \frac{A}{\sqrt{\nu}} - \frac{A}{\sqrt{\nu}} \sqrt{-\eta t_\eta} + \frac{1}{2} \frac{\lambda A}{\sqrt{\nu}} \frac{1}{\sqrt{-\eta t_\eta}}$$

$$- \frac{A \eta t_\eta}{6\sqrt{\nu}} + \frac{\frac{1}{2}A^2 - A^2 \log A + \mathcal{D}_1}{2A\nu} \frac{1}{\sqrt{-\eta t_\eta}} + \dots \quad . \qquad (1.5.63)$$

The transition expansion is

$$u = \frac{A}{\sqrt{\nu}} + \nu^{-5/6}\left[-A\sqrt{-\nu^{\frac{2}{3}}\eta t_\eta} + \dots\right]$$

$$+ \nu^{-7/6}\left[-\frac{1}{6} A \nu^{\frac{2}{3}} \eta t_\eta + \frac{1}{8} A \frac{\log(-\nu^{\frac{2}{3}}\eta t_\eta)}{\sqrt{-\nu^{\frac{2}{3}}\eta t_\eta}} + \dots\right] + \dots$$

$$= \frac{A}{\sqrt{-\nu}} - \frac{A}{\sqrt{\nu}} \sqrt{-\eta t_\eta} - \frac{1}{6} \frac{A}{\sqrt{-\nu}} \eta t_\eta + \frac{1}{8} A \frac{\frac{2}{3}\log \nu}{\nu^{\frac{2}{3}}\sqrt{-\eta t_\eta}} + \dots .$$

$$(1.5.64)$$

Comparison of (1.5.63) and (1.5.64) shows that it is necessary to choose $\frac{1}{12} A \nu^{-3/2} \log \nu = \frac{1}{2} \nu^{-\frac{1}{2}} \lambda A$, or $\lambda = \frac{1}{6} \frac{\log \nu}{\nu}$, and also $\mathcal{D}_1 = A^2 \log A - \frac{1}{2} A^2$.

The matching of the lower transition solution with the jump up occurs as $t^+ \to \omega_o$ and $\tilde{t} \to -\infty$. The intermediate limit is $\nu^{-1} << \eta << \nu^{-\frac{2}{3}}$, with $t_\eta < 0$ fixed and $\tilde{t} = \nu \eta t_\eta$. But since $t^+ = \nu^{\frac{2}{3}}(\hat{t} - \frac{1}{6} \frac{\log \nu}{\nu})$ and $\tilde{t} = \nu(\hat{t} - \chi(\nu))$, we have $\tilde{t} = \nu(\nu^{-\frac{2}{3}} t^+ + \frac{1}{6} \frac{\log \nu}{\nu} - \chi(\nu))$, and $t^+ - \omega_o =$

$\nu^{\frac{2}{3}}(\eta t_\eta + \zeta)$ where $\zeta(\nu) = \chi(\nu) - \frac{1}{6}\frac{\log\nu}{\nu} - \frac{\omega_o}{\nu^{\frac{2}{3}}}$. In the intermediate variables the transition expansion is

$$u = \frac{A}{\sqrt{\nu}} - \nu^{-5/6} A\left[\frac{1}{\nu^{\frac{2}{3}}(\eta t_\eta + \zeta)} - \tfrac{1}{3}\omega_o(\eta t_\eta + \zeta)\,\nu^{\frac{2}{3}} + \dots\right]$$

$$+ A\nu^{-7/6}\frac{\log(-\nu^{\frac{2}{3}}(\eta t_\eta + \zeta))}{\nu^{\frac{2}{3}}(\eta t_\eta + \zeta)^2} + \dots \qquad (1.5.65)$$

$$= \frac{A}{\sqrt{\nu}} - \frac{A}{\nu^{\frac{2}{3}}\eta t_\eta}\left(1 - \frac{\zeta}{\eta t_\eta} + \dots\right) + \frac{\frac{1}{3}\omega_o A}{\nu^{1/6}}(\eta t_\eta + \zeta) + \frac{\frac{2}{3}A\log\nu}{\nu^{5/2}(\eta t_\eta)^2} + \dots$$

The inner expansion is

$$u = \frac{A}{\sqrt{\nu}}\left\{1 + \frac{A}{\nu^{3/2}} + \dots - \frac{1 + \frac{4A}{\nu^{3/2}} + \dots)}{\nu\eta t_\eta}\right.$$

$$\left. + \frac{(1 + \frac{8A}{\nu^{3/2}} + \dots)\log(-\nu\eta t_\eta)}{(\nu\eta t_\eta)^2} + \dots\right\} + \qquad (1.5.66)$$

$$+ \mu_1(\nu)\,\mathcal{B}_1\left\{\frac{\nu\eta t_\eta}{3 + \dots} + \tfrac{2}{3}\left(1 + \frac{4A}{\nu^{3/2}} + \dots\right)\log(-\nu\eta t_\eta) + \dots\right\}$$

$$= \frac{A}{\sqrt{\nu}} - \frac{A}{\nu^{3/2}\eta t_\eta} + \frac{A\log\nu}{\nu^{5/2}(\eta t_\eta)^2} + \tfrac{1}{3}\mu_1(\nu)\mathcal{B}_1\nu\eta t_\eta + \dots .$$

To match (1.5.65) and (1.5.66) it is necessary to choose $\mu_1\nu = \nu^{1/6}$, that is $\mu_1(\nu) = \nu^{-7/6}$. Further, $\frac{1}{3}\omega_o A = \frac{1}{3}\mathcal{B}_1$, or $\mathcal{B}_1 = A\omega_o$. Also

$\frac{A\zeta}{\nu^{3/2}} = \frac{A\log\nu}{\nu^{5/2}}$, or $\zeta = \frac{\log\nu}{\nu}$. Thus $\chi(\nu) = \frac{7}{6}\frac{\log\nu}{\nu} + \frac{\omega_o}{\nu^{\frac{2}{3}}}$. This choice of $\mathcal{B}_1$ means that (1.5.36) becomes

$$z_1 = A\omega_o\left(1 + \frac{4A}{\nu^{3/2}} + \frac{19A^2}{\nu^3} + \ldots\right) + \text{TST},$$

as $\tilde{t} \to +\infty$.

The only matching remaining to be done is that of the jump down to the lower outer solution and the jump up to the upper outer solution. First it will be necessary to calculate the expansion of the lower outer solution at the bottom of the jump down; this had been postponed earlier.

To leading order, it was found that as $\hat{t} \to -t_j$,

$$w_o = \frac{4A^2}{\nu^{3/2}}\left(1 - \frac{8A^2}{\nu^3} + \ldots\right).$$

We expand (1.5.13) about this value of $w_o$ and obtain

$$w_o = \frac{4A^2}{\nu^{3/2}}\left(1 - \frac{8A^2}{\nu^3} + \ldots\right)$$
$$+ \frac{4A^2}{\nu^{3/2}}\left(1 + \frac{24A^2}{\nu^3} + \ldots\right)[\hat{t} + \tfrac{3}{2}\log\nu - \log A - 2\log 2 + O(\nu^{-3})] + \ldots \tag{1.5.67}$$

Expansion of (1.5.14) about the same value of $w_o$ yields

$$w_1 = \frac{1}{A^2}\left(1 + \frac{16A^2}{\nu^3} + \ldots\right)\left\{\frac{4A^2\mathcal{D}_1}{\nu^{3/2}}\left(1 - \frac{8A^2}{\nu^3} + \ldots\right)\right.$$
$$\left. -A^2\left(1 - \frac{8A^2}{\nu^3} + \ldots\right)\frac{4A^2}{\nu^{3/2}}[-\tfrac{3}{2}\log\nu + \log 4A^2 - \frac{8A^2}{\nu^3} + \ldots] + \ldots\right\} + \ldots$$
$$= \left(1 + \frac{16A^2}{\nu^3} + \ldots\right)\left\{6A^2\frac{\log\nu}{\nu^{3/2}} + \frac{1}{\nu^{3/2}}(4\mathcal{D}_1 - 4A^2\log 4A^2)\right.$$
$$\left. + O(\nu^{-9/2})\right\} + \ldots \tag{1.5.68}$$

The limit to be taken in matching the lower outer solution and the jump down is $\bar{t} \to +\infty$, $t \to 0+$. We have $\bar{t} = \nu(t-\theta_o)$ and $\hat{t} = t - t_j$, so $\bar{t} = \nu(\hat{t} + t_j - \theta_o)$. We let $\bar{t} = \nu\eta t_\eta$ where $\nu^{-1} \ll \eta \ll 1$ and $t_\eta > 0$ is fixed, so that $\hat{t} = \eta t_\eta - t_j + \theta_o$. In the intermediate variables the inner expansion is just

$$u = \frac{4A^2}{\nu^2}\left(1 - \frac{8A^2}{\nu^3} + \ldots\right) - \frac{16A^2}{\nu^4}(A^{4/3}\,\omega_o) + \text{TST}\,, \qquad (1.5.69)$$

and the outer expansion is

$$u = \frac{4A^2}{\nu^2}\left(1 - \frac{8A^2}{\nu^3} + \ldots\right) + \frac{4A^2}{\nu^2}\left(1 + \frac{24A^2}{\nu^3} + \ldots\right)$$

$$\times\left[\eta t_\eta - t_j + \theta_o + \frac{3}{2}\log\nu - \log A - 2\log 2 + O(\nu^{-3})\right] + \ldots +$$

$$+ \frac{1}{\nu}\left(1 + \frac{16A^2}{\nu^3} + \ldots\right)\left[6A^2\,\frac{\log\nu}{\nu^{3/2}} + \frac{1}{\nu^{3/2}}(-4A^2\log A\right.$$

$$\left. -A^2(2-8\log 2)) + \ldots\right] + \ldots \;. \qquad (1.5.70)$$

In order to match these expansions we must pick

$$t_j = \theta_o + \frac{3}{2}\log\nu - \log A - 2\log 2$$

$$+ \frac{3}{2}\,\frac{\log\nu}{\nu^{\frac{1}{2}}} - \frac{1}{4}(4\log A + (2-8\log 2))\,\frac{1}{\nu^{\frac{1}{2}}} + \ldots \;. \qquad (1.5.71)$$

The matching is then correct up to order $\nu^{-5/2}\log\nu$; the first omitted term in equation (1.5.71) is of order $\nu^{-3}\log\nu$. The error in $t_j$ is smaller than order $\nu^{-\frac{1}{2}}$.

The final matching is of the jump up to the upper outer solution. The jump up ends at $u = \nu^{-\frac{1}{2}}\psi + O(\nu^{-7/6})$; in intermediate variables this is just

$$u = \nu\left(1 - \frac{2A}{\nu^{3/2}} - \frac{2A^2}{\nu^3} + \dots\right) + O(\nu^{-7/6}) + \text{TST} \;, \qquad (1.5.72)$$

and so the outer solution is to be expanded about $u_o = 1 - \frac{2A}{\nu^{3/2}} - \frac{2A^2}{\nu^3} + \dots$ . However, this portion of the cycle is no longer given by (1.5.8) but by the expression

$$-(u_o - \tfrac{1}{2})^2 = A^2\bar{\tau} \;,$$

where $\bar{\tau} = \nu^{-2}(\tau - T(\nu))$ and $T(\nu)$ is the period of the oscillation. The outer limit has $\bar{\tau}$ fixed. The variable $u_o$ takes on the proper value when

$$\bar{\tau} = \bar{\tau}_o = -\frac{1}{4A^2}\left(1 - \frac{8A}{\nu^{3/2}} + \frac{8A^2}{\nu^3} + \dots\right) .$$

The expansion of $u_o$ is therefore

$$u_o = 1 - \frac{2A}{\nu^{3/2}} + \dots + A_1\left(\bar{\tau} + \frac{1}{4A^2}\left[1 - \frac{8A}{\nu^{3/2}} + \dots\right]\right)$$

$$+ A_2\left(\bar{\tau} + \frac{1}{4A^2}\left[1 - \frac{8A}{\nu^{3/2}} + \dots\right]\right)^2 + \dots \;,$$

where

$$A_1 = \left.\frac{du_o}{d\bar{\tau}}\right|_{\bar{\tau}=\bar{\tau}_o} = -A^2\left(1 + \frac{4A}{\nu^{3/2}} + \dots\right) \;,$$

$$A_2 = \left.\frac{d^2u_o}{d\bar{\tau}^2}\right|_{\bar{\tau}=\bar{\tau}_o} = -2A^4\left(1 + \frac{12A}{\nu^{3/2}} + \dots\right) .$$

Then

$$u_1 = \frac{1}{u_o - \frac{1}{2}} \left\{ -u_o + \tfrac{1}{2}\log u_o + \tfrac{1}{2}(1+\log 2) \right\}$$

$$= (\log 2 - 1 + \frac{2A}{\nu^{3/2}} + \ldots)(1 + \frac{4A}{\nu^{3/2}} + \ldots) + \ldots \quad .$$

Now $t = \bar{\tau}\nu^2 + T(\nu)$ and

$$\tilde{t} = \nu(\hat{t} - \chi(\nu))$$

$$= \nu(t - t_j - \frac{7}{6}\frac{\log\nu}{\nu} - \frac{\omega_o}{\nu^{2/3}})$$

$$= \nu(t - \frac{\omega_o}{A^{2/3}} - \frac{3}{2}\log\nu + \log A + 2\log 2 + \ldots) \quad .$$

Thus

$$\tilde{t} = \nu(\bar{\tau}\nu^2 + T(\nu) - \frac{3}{2}\log\nu + \log A - \frac{\omega_o}{A^{\frac{2}{3}}} + 2\log 2 + \ldots) \quad .$$

We choose the intermediate limit $\nu^{-1} \ll \eta \ll \nu^2$, where $\tilde{t} = \nu\eta t_\eta$ and $t_\eta$ is fixed. Thus

$$\bar{\tau}\nu^2 = \eta t_\eta - T(\nu) + \frac{3}{2}\log\nu - \log A + \frac{\omega_o}{A^{2/3}} - 2\log 2 + \ldots \quad .$$

In the intermediate variables the outer expansion is

$$u = \nu\left(1 - \frac{2A}{\nu^{3/2}} + \ldots\right) - \nu A^2 \left(1 + \frac{4A}{\nu^{3/2}} + \ldots\right)$$
$$\times \left\{ \frac{\eta t_\eta}{\nu^2} - \frac{T(\nu) - \frac{3}{2}\log\nu + \log A - A^{-\frac{2}{3}}\omega_o + 2\log 2}{\nu^2} + \right. \qquad (1.5.73)$$
$$\left. + \frac{1}{4A^2}\left(1 - \frac{8A}{\nu^{3/2}} + \ldots\right)\right\} + \ldots + \left(\log 2 - 1 + \frac{2A}{\nu^{3/2}} + \ldots\right)$$
$$\times \left(1 + \frac{4A}{\nu^{3/2}} + \ldots\right) \quad .$$

In order to match (1.5.72) and (1.5.73) we choose

$$T(\nu) = \frac{\nu^2}{4A^2}\left(1 - \frac{8A}{\nu^{3/2}} + \dots\right) + \frac{3}{2}\log\nu - \log A$$

$$+ \frac{\omega_o}{A^{\frac{2}{3}}} - 2\log 2 + \frac{\nu}{A^2}(1-\log 2) \;.$$

The error made in $T(\nu)$ by omitting other terms in $u_o$ and $u_1$ is $O(\nu^{-1})$, while the error made by omitting $u_2$ is O(1).

Summary

The more detailed description of the solution of (1.5.3) is now given by the equations (1.5.8), (1.5.9), (1.5.39), (1.5.46), (1.5.22), (1.5.27), (1.5.13), (1.5.14), (1.5.51), (1.5.55), (1.5.31), and (1.5.34), together with the values of the integration constants that were found from the matching. It is clear how the calculation could be continued if it were desired.

For the values $\nu = 78$, $A = 8.2$, $\omega_o = 2.338$ we calculate $T(\nu) = 24.5$. Lavenda, Nicolis, and Herschkowitz-Kaufman [6] calculate T = 24.3 asymptotically and T = 25.3 numerically. It seems clear that it is not $\nu$ alone, but some combination of $\nu$ and A that is the proper large parameter in this problem. However, A enters into the formulae for $T(\nu)$ and u in a very complicated way, and it is not clear what the combination should be. The fact that the error made in $T(\nu)$ by omitting $u_2$ is O(1) indicates that it is partly good luck that the asymptotic values of T agree as well as they do with the real value. The other number that the authors calculate in [6] is the maximum of $X = A/u$. This corresponds to the bottom of the jump down, which is given by (1.5.62) as

$$u_{min} = \frac{4A^2}{\nu^2}\left(1 - \frac{4A^{4/3}\omega_o}{\nu^2} - \frac{8A^2}{\nu^3} + \ldots\right) .$$

Thus

$$X_{max} = \frac{\nu^2}{4A}\left(1 + \frac{4A^{4/3}\omega_o}{\nu^2} + \frac{8A^2}{\nu^3} + \ldots\right) = 190.5 .$$

Lavenda, Nicolis, and Herschkowitz-Kaufman calculate $X_{max} = 189$ numerically.

## 2. Localized Disturbances

The analysis of the rate equations in the case that the concentration of the reactant A is not constant is made considerably more difficult by the fact that the basic steady state is no longer uniform. However, the principles will be the same as those of the last chapter. The basic state may be stable or unstable, depending on the parameters $A(r)$, B, D, and $\delta$. The neutral stability curve in the $\delta$, B plane will be similar to figure 1.1.3. It will have two portions, one of which occurs when the eigenvalue of the linearized stability problem with the greatest real part has real part zero and imaginary part non-zero, and the other of which occurs when the eigenvalue with the greatest real part is purely real. If the point $\delta$, B is slightly above the neutral stability curve and in a region corresponding to region III of figure 1.1.3, we expect to see the bifurcation of a time-periodic disturbance. If $\delta$, B is slightly above the neutral stability curve but in a region corresponding to region II of figure 1.1.3, we expect the bifurcation of a new steady state. Just as in sections 1.2 and 1.4, these disturbances should be multiples of the eigenfunctions corresponding to the eigenvalues with the greatest real parts.

The question of the localization of disturbances when the basic state is slightly unstable is therefore intimately related to that of the form of the eigenfunctions of the linearized stability problem. Since the equations of linearized stability have variable coefficients and the boundary value problem for eigenfunctions is not self-adjoint, the calculation of the eigenvalues and eigenfunctions is very difficult in general. However, when the diffusion coefficients are small it is possible to obtain some information by the WKBJ technique.

## 2.1. The Basic State and its Stability

The equations to be studied in this chapter are (0.2.1) and (0.2.2), namely

$$\frac{\partial X}{\partial t} = A(r) - (B+1)X + X^2Y + D\frac{\partial^2 X}{\partial r^2} , \tag{0.2.1}$$

$$\frac{\partial Y}{\partial t} = BX - X^2Y + \mathcal{S}D\frac{\partial^2 Y}{\partial r^2} . \tag{0.2.2}$$

D is a small quantity and $\mathcal{S} = O(1)$. The function A(r) varies slowly compared with the length scale $D^{\frac{1}{2}}$. It is given explicitly by

$$A(r) = \overline{A} \operatorname{sech} \frac{1}{2\sqrt{D_A}} \cosh \frac{r-\frac{1}{2}}{\sqrt{D_A}} . \tag{2.1.1}$$

The boundary conditions are $X(0,t) = X(1,t) = \overline{A}$ and $Y(0,t) = Y(1,t) = B/\overline{A}$.

Under these conditions, there is a basic steady state $X_o(r)$, $Y_o(r)$ which may be found asymptotically by a regular perturbation expansion in the small parameter D. (There are no boundary layers because the boundary conditions have been fixed in such a manner that the basic state automatically satisfies them.) The expansion is

$$X_o \sim A(r) + D\left(A''(r) + \mathcal{S}B\left(\frac{1}{A(r)}\right)''\right) + O(D^2) , \tag{2.1.2}$$

$$Y_o \sim \frac{B}{A(r)} + D\left(-BA''(r) - (B-1)\mathcal{S}B\left(\frac{1}{A(r)}\right)''\right)\frac{1}{A^2(r)} + O(D^2) . \tag{2.1.3}$$

Just as in section 1.1, we find the equations of linearized stability for $X_o$ and $Y_o$ by writing $X = X_o+u$, $Y = Y_o+v$, substituting into (0.2.1) and (0.2.2), and neglecting the non-linear terms. The linearized stability equations are

$$\frac{\partial u}{\partial t} = \left[-(B+1) + 2X_oY_o\right] u + X_o^2 \, v + D \frac{\partial^2 u}{\partial r^2} , \tag{2.1.4}$$

$$\frac{\partial v}{\partial t} = \left[B - 2X_oY_o\right] u - X_o^2 \, v + \vartheta D \frac{\partial^2 v}{\partial r^2} , \tag{2.1.5}$$

together with the boundary conditions $u(0,t) = u(1,t) = v(0,t) = v(1,t) = 0$. If we look for solutions of the form $u = e^{\sigma t} \phi(r)$, $v = e^{\sigma t} \psi(r)$, we find that the equations for $\phi$ and $\psi$ are

$$\sigma\phi = \left[-(B+1) + 2X_oY_o\right] \phi + X_o^2 \, \psi + D\phi'', \tag{2.1.6}$$

$$\sigma\psi = \left[B-2X_oY_o\right] \phi - X_o^2 \, \psi + \vartheta D\psi'' , \tag{2.1.7}$$

and the boundary conditions are $\phi(0) = \phi(1) = \psi(0) = \psi(1) = 0$. (These equations reduce to (1.1.5) and (1.1.6) if A is constant and $X_o \equiv A$, $Y_o \equiv B/A$.)

Since the coefficients of (2.1.6) and (2.1.7) are variable and the system is not self-adjoint, we cannot expect to solve this eigenvalue problem exactly. However, it is possible to take advantage of the facts that D is small and that the coefficients vary slowly compared with a length scale $D^{\frac{1}{2}}$. In the next section we use the WKBJ technique to consider (2.1.6) and (2.1.7).

## 2.2. Possibility of Localization

The stability of the basic steady state is determined by the eigenvalues of the boundary value problem

$$\sigma\phi = [-(B+1) + 2X_o Y_o]\,\phi + X_o^2\psi + D\phi'' , \qquad (2.1.6)$$

$$\sigma\psi = [B-2X_o Y_o]\,\phi - X_o^2\psi + \vartheta D\psi'' , \qquad (2.1.7)$$

with boundary values $\phi(0) = \phi(1) = \psi(0) = \psi(1) = 0$. The form of the solution when the basic state is slightly unstable is determined by the eigenfunctions of the problem. In this section we use the WKBJ technique to investigate the eigenfunctions, and show how the localization of disturbances can arise out of the presence of turning points.

We seek solutions to (2.1.6) and (2.1.7) of the form

$$\begin{bmatrix} \phi \\ \\ \psi \end{bmatrix} \sim \exp \frac{iw(r)}{\sqrt{D}} \left\{ \begin{bmatrix} f_o(r) \\ \\ g_o(r) \end{bmatrix} + \sqrt{D} \begin{bmatrix} f_1(r) \\ \\ g_1(r) \end{bmatrix} + D \begin{bmatrix} f_2(r) \\ \\ g_2(r) \end{bmatrix} + \ldots \right\} . \qquad (2.2.1)$$

Substitution of this expansion into the equations (2.1.6) and (2.1.7), and equation of coefficients of powers of $\sqrt{D}$ to zero, produces the following hierarchy of equations:

$$\begin{bmatrix} \sigma + w'^2 + (B+1) - 2X_o Y_o & -X_o^2 \\ \\ -B + 2X_o Y_o & \sigma + \vartheta w'^2 + X_o^2 \end{bmatrix} \begin{bmatrix} f_o \\ \\ g_o \end{bmatrix} = \begin{bmatrix} 0 \\ \\ 0 \end{bmatrix} ; \qquad (2.2.2)$$

$$\begin{bmatrix} \sigma+w'^2+(B+1)-2X_oY_o & -X_o^2 \\ -B+2X_oY_o & \sigma+\vartheta w'^2+X_o^2 \end{bmatrix}\begin{bmatrix} f_1 \\ g_1 \end{bmatrix} = \begin{bmatrix} i(w''f_o+2w'f_o') \\ \vartheta i(w''g_o+2w'g_o') \end{bmatrix} . \quad (2.2.3)$$

The system (2.2.2) is homogeneous. Thus it will have a solution only if the rows of the matrix operating on $[f_o, g_o]^t$ are linearly dependent, so that the determinant of the coefficients is zero. Suppose that the sum of the first row and c times the second row is zero. Then by adding c times the second equation to the first equation in each of (2.2.2) and (2.2.3), we obtain the following systems:

$$\begin{bmatrix} 0 & 0 \\ -B+2X_oY_o & \sigma+\vartheta w'^2+X_o^2 \end{bmatrix}\begin{bmatrix} f_o \\ g_o \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (2.2.4)$$

and

$$\begin{bmatrix} 0 & 0 \\ -B+2X_oY_o & \sigma+\vartheta w'^2+X_o^2 \end{bmatrix}\begin{bmatrix} f_1 \\ g_1 \end{bmatrix} = \begin{bmatrix} i[w''(f_o+c\vartheta g_o)+2w'(f_o'+c\vartheta g_o')] \\ \vartheta i(w''g_o+2w'g_o') \end{bmatrix} . \quad (2.2.5)$$

From (2.2.4) we obtain the relation

$$(-B+2X_oY_o)\, f_o + (\sigma+\vartheta w'^2+X_o^2)g_o = 0 \quad , \quad (2.2.6)$$

and from (2.2.5) the differential equation

$$w''(f_o + c\vartheta g_o) + 2w'(f_o + c\vartheta g_o)' = 0 \quad . \tag{2.2.7}$$

The phase function w(r) is to be found from the equation

$$\det \begin{bmatrix} \sigma + w'^2 + (B+1) - 2X_oY_o & -X_o^2 \\ \\ -B + 2X_oY_o & \sigma + \vartheta w'^2 + X_o^2 \end{bmatrix} = 0 \tag{2.2.8}$$

by solving the quartic and integrating. With w(r) known, equation (2.2.7) integrates to

$$(f_o + c\vartheta g_o)\sqrt{w'} = \text{const}, \tag{2.2.9}$$

where the principal branch of the square root is taken. Then (2.2.6) and (2.2.9) yield

$$g_o = \frac{\text{const}}{\sqrt{w'}} \left[ c\vartheta + \frac{\sigma + \vartheta w'^2 + X_o^2}{B - 2X_oY_o} \right]^{-1} , \tag{2.2.10}$$

so that $f_o$ and $g_o$ are determined up to constants. Some of the constants are determined by imposing the boundary conditions at r = 0. The boundary conditions at r = 1 can be satisfied only for certain values of σ, which are the eigenvalues of the problem.

This procedure works only if the term

$$c\vartheta + \frac{\sigma + \vartheta w'^2 + X_o^2}{B - 2X_oY_o}$$

in (2.2.10) does not vanish. If it does, then $f_o$ and $g_o$ are infinite, so that the asymptotic approximation (2.2.1) breaks down there. This difficulty is equivalent to the phenomenon of turning points familiar in quantum mechanics. Since from (2.2.8)

$$\sigma + w'^2 + (B+1) - 2X_oY_o = c\,[B-2X_oY_o] ,$$

the condition that (2. 2. 1) be valid is

$$\vartheta\,[\sigma + w'^2 + (B+1) - 2X_oY_o] + \sigma + \vartheta w'^2 + X_o^2 \neq 0 ,$$

i. e.,

$$2\vartheta w'^2 + \vartheta\,[\sigma+(B+1)-2X_oY_o] + \sigma + X_o^2 \neq 0 . \qquad (2.2.11)$$

But the solution to (2. 2. 8) is

$$\begin{aligned} 2\vartheta w'^2 = &- \left\{\vartheta\,[\sigma+(B+1) - 2X_oY_o] + \sigma + X_o^2\right\} \\ &\pm \left[\left\{\vartheta\,[\sigma+(B+1)-2X_oY_o] + \sigma + X_o^2\right\}^2 \right. \\ &\left. -4\vartheta\left\{\sigma\,[\sigma+(B+1)+X_o^2 - 2X_oY_o] + X_o^2\right\}\right]^{\frac{1}{2}} . \end{aligned} \qquad (2.2.12)$$

Comparing (2. 2. 11) and (2. 2. 12), we see that the asymptotic approximation (2. 2. 1) breaks down exactly where the discriminant of (2. 2. 8) vanishes; that is, where

$$\begin{aligned} &\left\{\vartheta\,[\sigma+(B+1) - 2X_oY_o] + \sigma + X_o^2\right\}^2 \\ &= 4\vartheta\left\{\sigma\,[\sigma+(B+1) + X_o^2 - 2X_oY_o] + X_o^2\right\} . \end{aligned} \qquad (2.2.13)$$

It is of particular interest to find the locations of the points where the discriminant vanishes in the case $\sigma = 0$. This will correspond to a value $B = B_c$, the point of neutral stability in the $\vartheta$, B plane for an eigenfunction. Equation (2. 2. 13) becomes

$$\left[\vartheta\left[(B_c+1) - 2X_oY_o\right] + X_o^2\right]^2 = 4\vartheta X_o^2 .$$

In terms of $X_o = A(r) + O(D)$ and $Y_o = \frac{B_c}{A(r)} + O(D)$, this is

$$[\vartheta(-B_c+1) + A^2(r)]^2 = 4\vartheta A^2(r) + O(D) ,$$

or

$$B_c = 1 - \frac{2A(r)}{\sqrt{\vartheta}} + \frac{A^2(r)}{\vartheta} + O(\sqrt{D}) . \qquad (2.2.14)$$

(In taking the square root we have assumed that $\vartheta(-B_c+1) + A^2(r)$ is positive. This will be justified shortly.) Let the maximum and minimum values of $A(r)$ be $\overline{A}$ and $A_{min}$, respectively. Then the asymptotic approximation (2.2.1) for an eigenfunction corresponding to $\sigma = 0$ and $B = B_c$ will not be valid in the entire interval $0 \leqslant r \leqslant 1$ if $B_c$ is such that

$$\left(1 - \frac{A_{min}}{\sqrt{\vartheta}}\right)^2 < B_c < \left(1 - \frac{\overline{A}}{\sqrt{\vartheta}}\right)^2 .$$

(The term $O(\sqrt{D})$ has been omitted in writing down this inequality.) A picture of the function $(1 - A/\sqrt{\vartheta})^2$ together with a possible value of $B_c$ is given in figure 2.2.1. Call the values of r for which (2.2.14) holds $r_1$ and $r_2$. Then for $r_1 < r < r_2$, $B_c > \left(1 - \frac{A}{\sqrt{\vartheta}}\right)^2$ while for $0 \leqslant r \leqslant r_1$ and $r_2 < r \leqslant 1$, $B_c < \left(1 - \frac{A}{\sqrt{\vartheta}}\right)^2$.

Next we consider the approximation (2.2.1) in the regions $r_1 < r < r_2$ and $0 \leqslant r < r_1$, $r_2 < r \leqslant 1$. Equation (2.2.12) for the case $\sigma = 0$ is

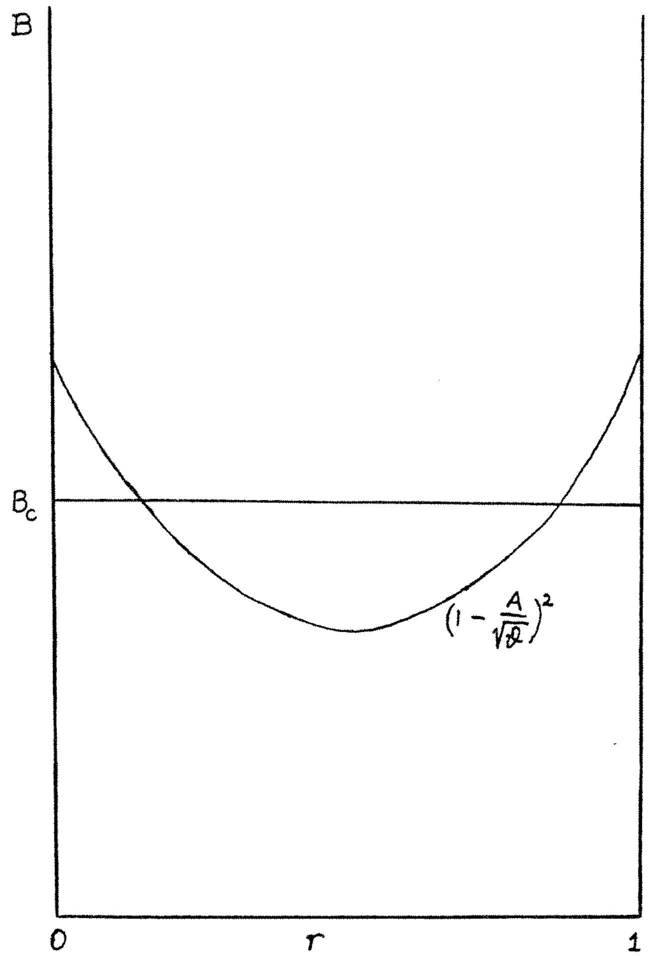


Figure 2. 2. 1. A possible value of B for a localized disturbance. The exponential exp $\frac{iw(r)}{\sqrt{D}}$ is oscillatory when $B_c$ lies above the curve $(1 - A/\sqrt{\mathcal{D}})^2$.

$$2\vartheta w'^2 = -\{\vartheta[-B_c+1] + A^2(r)\} \pm [\{\vartheta[-B_c+1] + A^2(r)\}^2 - 4\vartheta A^2(r)]^{\frac{1}{2}} . \qquad (2.2.15)$$

It is seen that if $\vartheta[-B_c+1] + A^2(r) = 0$, then $w'^2$ is complex. Thus the points where $B_c = 1 + \frac{A^2}{\vartheta}$ must lie to the left of $r_2$ and to the right of $r_1$. This would not occur if we chose $B_c = \left(1 + \frac{A}{\sqrt{\vartheta}}\right)^2$ instead of (2.2.14) as the points where (2.2.1) ceases to be valid.

It is also seen from (2.2.15) that those portions of the curve $\left(1 - \frac{A}{\sqrt{\vartheta}}\right)^2$ which lie above $B_c$ correspond to $w'^2 < 0$. Thus the exponential

$$\exp \frac{iw(r)}{\sqrt{D}}$$

is not oscillatory in such regions. If $B < \left(1 - \frac{A_{min}}{\sqrt{\vartheta}}\right)^2$, the curve lies entirely above B and the exponential is non-oscillatory across the entire interval $0 \leqslant r \leqslant 1$. In such a case it is impossible to satisfy homogeneous boundary conditions at both ends. Thus no new steady state can be excited at a value of B which is less than $1 - \frac{2A_{min}}{\sqrt{\vartheta}} + \frac{A_{min}^2}{\vartheta}$. We conclude that the portion of the neutral stability curve in the $\vartheta$, B plane that is obtained by the consideration of real eigenvalues, must lie above the curve

$$B = 1 - \frac{2A_{min}}{\sqrt{\vartheta}} + \frac{A_{min}^2}{\vartheta} .$$

(This result might be compared with the exact result of section 1.1. There the neutral stability curve for the uniform solution was given by

$$B = \min_n \left\{ 1 + \frac{A^2}{\vartheta} + n^2\pi^2 D + \frac{A^2}{\vartheta(n^2\pi^2 D)} \right\} \quad . )$$

If $B_c$ lies above $(1 - \frac{\overline{A}}{\sqrt{\vartheta}})^2$, then $w'^2$ is complex across the entire interval, so that the exponential $\exp \frac{iw(r)}{\sqrt{D}}$ is always oscillatory. Eigenfunctions corresponding to values $B = B_c$ in this region are therefore not localized, and correspond closely to the eigenfunctions $\underline{\phi}_n^{\pm} = [\sin n\pi r,\ M_n^{\pm} \sin n\pi r]^t$ of chapter 1.

Finally, if $B_c$ satisfies

$$\left(1 - \frac{A_{min}}{\sqrt{\vartheta}}\right)^2 < B_c < \left(1 - \frac{\overline{A}}{\sqrt{\vartheta}}\right)^2 ,$$

then there are values $r_1$ and $r_2$ for which (2.2.14) is satisfied. For $r_1 < r < r_2$, the exponential $\exp \frac{iw(r)}{\sqrt{D}}$ is oscillatory; for $0 \leq r < r$, and $r_2 < r \leq 1$ it is not. Eigenfunctions corresponding to values $B = B_c$ in this region are therefore localized. The mechanism of localization is the change from negative to complex of the function $(w'(r))^2$, and that occurs because $A(r)$ varies.

## 3. Conclusions

The equations describing Prigogine's model reaction show unexpected mathematical richness, and the results of the previous chapters are only a step towards understanding them. However, a few conclusions may be drawn at this stage.

Nicolis and Auchmuty [12] have argued that the bifurcation of non-uniform steady states forms a basis for understanding the mechanism of biological pattern formation, and specifically morphogenesis. We are not so sure. It would seem reasonable that the formation of biological structures is a result of repeated loss of stability and branching. More and more complicated structures would appear at each point of secondary bifurcation. The equations studied in section 1.3 do not exhibit secondary bifurcation, and it is our opinion that the full equations (with both $D_X$ and $D_Y$ finite) do not show it either. If that is the case, then the range of patterns that the model can exhibit is limited, and so is the model's utility as an explanation of morphogenesis. The mechanism of pattern formation in biology is undoubtedly extremely complicated; and it seems unlikely that consideration of only reaction and diffusion is sufficient to explain it in more than the most primitive cases.

The phenomenon of localization studied in chapter 2 is evidently a consequence of the simplifying assumptions made in arriving at equations (0.2.1) and (0.2.2). Since both A and B are the initial reactants, there is no particular reason (aside from simplifying the equations enough to make them tractable) to assume that B is to be uniformly distributed when A is not. In this respect, then, the localized disturbance is artificial. However, if the equation for the concentration of B is considered, it is found that there is no uniform solution of the partial differential equations for which all the concentrations are positive. Hence, if a non-uniform solution of the equations is unstable, the new disturbance may be localized in the sense that the leading eigenfunction of the linearized stability problem may have parts that are oscillatory and non-oscillatory in space.

The model appears to be more relevant to the study of chemical waves and oscillations, since these have been observed experimentally (see [14] and [15]) under conditions in which only reaction and diffusion are likely to be operating. It should be noted that the waves studied in section 1.5 are only kinematic, since the oscillations at each point in space are not coupled. Also, these oscillations cannot satisfy the boundary conditions. However, they might serve as a candidate for the first term in the outer expansion (away from the boundaries) for time-periodic solutions of (1.1.1) and (1.1.2) in the case that diffusion is small in the special circumstances that the initial conditions are sufficiently smooth that the derivative $\frac{\partial^2 X_o(t-\eta(r))}{\partial r^2}$ is O(1). Then (1.1.1) and (1.1.2) are satisfied to O(D). If that is not the case, and near the boundaries, it becomes necessary to include the diffusion terms explicitly.

## Appendix. On the Signs of Coefficients Appearing in the Formulae for Bifurcating Solutions

Certain expressions appear in equation (1.2.14) whose sign is not obvious. They can be determined by consideration of the definitions of $M_N^+$ and $B_c$.

We had for the bifurcation of steady states,

$$B_c = 1 + N^2\pi^2 D + \frac{A^2}{\vartheta}\left(1 + \frac{1}{N^2\pi^2 D}\right) ,$$

and in general

$$A^2 M_n^{\pm} = \sigma_n^{\pm} - (B-1) + n^2\pi^2 D .$$

If $\sigma_N^+ = 0$ then

$$A^2 M_N^+ = -(B_c - 1) + N^2\pi^2 D$$

$$= -\frac{A^2}{\vartheta}\left(1 + \frac{1}{N^2\pi^2 D}\right) .$$

Thus

$$1 + \frac{A^2}{B_c} M_N^+ = \frac{1}{B_c}\left[1 + N^2\pi^2 D + \frac{A^2}{\vartheta}\left(1 + \frac{1}{N^2\pi^2 D}\right) - \frac{A^2}{\vartheta}\left(1 + \frac{1}{N^2\pi^2 D}\right)\right]$$

$$> 0 .$$

Also, if $\sigma_N^+ = 0$ then $\sigma_N^- < 0$; using $M_N^+ M_N^- = \frac{B_c}{A^2}$ we find

$$1 - \frac{A^2}{B_c}(M_N^+)^2 = 1 - \frac{M_N^+}{M_N^-}$$

$$= 1 - \frac{-(B_c - 1) + N^2\pi^2 D}{\sigma_N^- - (B_c - 1) + N^2\pi^2 D}$$

$$> 0 \ .$$

The third quantity whose sign is to be considered is

$$\frac{B_c}{A} + 2AM_N^+ = \frac{B_c}{A}\left(1 + \frac{2A^2}{B_c}\, M_N^+\right)$$

$$= \frac{1}{A}\left[1 + N^2\pi^2 D - \frac{A^2}{\vartheta}\left(1 + \frac{1}{N^2\pi^2 D}\right)\right].$$

From (1.1.14) we see that N = 1 corresponds to

$$\vartheta \geqslant \frac{A^2}{4(\pi^2 D)^2} \ ,$$

while other values of N correspond to

$$\frac{A^2}{N^2(N+1)^2(\pi^2 D)^2} \leqslant \vartheta \leqslant \frac{A^2}{(N-1)^2 N^2(\pi^2 D)^2} \ .$$

Thus for $N \neq 1$

$$(1+N^2\pi^2 D)(1-(N+1)^2\pi^2 D) \leqslant A\left(\frac{B_c}{A} + 2AM_N^+\right)$$

$$\leqslant (1+N^2\pi^2 D)(1-(N-1)^2\pi^2 D) \ ,$$

and as $\vartheta$ changes, the quantity $A(\frac{B_c}{A} + 2AM_N^+)$ takes on all the intermediate values. Hence the quantity

$$\frac{B_c}{A} + 2AM_N^+$$

may change sign as $\vartheta$ changes; it will if $1-(N-1)^2\pi^2 D > 0$ but $1-(N+1)^2\pi^2 D < 0$.

The quantity

$$\frac{B_c}{A} + 2AM_{N+1}^{+}$$

will change sign if $1-N^2\pi^2D > 0$ but $1-(N+2)^2\pi^2D < 0$, and $\frac{B_c}{A} + 2AM_{N-1}^{+}$ will change sign if $1-(N-2)^2\pi^2D > 0$ but $1-N^2\pi^2D < 0$. Thus there are at most two values of N for which the expression $\frac{B_c}{A} + 2AM_N^{+}$ changes sign in the interior of an interval

$$\frac{A^2}{N^2(N+1)^2(\pi^2D)^2} \leqslant \vartheta \leqslant \frac{A^2}{(N-1)^2N^2(\pi^2D)^2} \;.$$

For very large values of $\vartheta$, the expression is positive.

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