AD-A087 114 CENTER FOR NAVAL ANALYSES ALEXANDRIA VA OPERATIONS EV--ETC F/G 7/4

LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS.(U)

JUN 80 D COPE

UNCLASSIFIED OEG-PP-287 NL

1 OF 4

AD A 087114

PROFESSIONAL PAPER 287 / June 1980

LEVEL II

LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS

Davis Cope

AD A087114

DTIC ELECTE JUL 24 1980 D

C

This document has been approved for public release and sale; its distribution is unlimited.

CNA

CENTER FOR NAVAL ANALYSES

2000 North Beauregard Street, Alexandria, Virginia 22311

DDC FILE COPY

80 7 23 090

DTIC
ELECTE
JUL 24 1980
D
C

9 PROFESSIONAL PAPER 287 Jun[redacted]80 11

16 # LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS.

10 Davis Cope

Dissertation submitted to the faculty of the Graduate School of Vanderbilt University in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mathematics, August, 1980, Nashville, Tennessee.

12 331

14 OEG-PP-287

This document has been approved for public release and sale; its

Operations Evaluation Group
CENTER FOR NAVAL ANALYSES
2000 North Beauregard Street, Alexandria, Virginia 22311

270700 Gm

LIMIT CYCLE SOLUTIONS OF

REACTION-DIFFUSION EQUATIONS

by

Davis Cope

Dissertation

Submitted to the Faculty of the

Graduate School of Vanderbilt University

in partial fulfillment of the requirements

for the degree of

DOCTOR OF PHILOSOPHY

in

MATHEMATICS

August, 1980

Nashville, Tennessee

Accession For
NTIS GRA&I
DDC TAB
Unannounced
Justification Per form
50 on file
By
Distribution/
Availability Codes
Dist | Avail and/or special
A

Approved: Date:

ACKNOWLEDGEMENTS

Many people have generously helped in the completion of this thesis. There is not space to mention them all here, but I would especially like to thank the following:

Robert Miura was my thesis advisor at Vanderbilt and then at the University of British Columbia, and I appreciate his support and suggestions throughout the work on this thesis.

The Department of Mathematics of the University of British Columbia extended its hospitality to me as a visiting graduate student while the research of this thesis was completed.

An American Mathematical Society grant enabled me to attend the 1978 AMS-SIAM meeting on Nonlinear Oscillations in Biology. In particular, conversations there with Art Winfree of Purdue University and Jack Hale of Brown University were helpful in the work for Chapter III.

Neil Fenichel has shown me how geometric concepts from the theory of dynamical systems can be used to give particularly vivid descriptions of behavior in reaction-diffusion systems.

Jim Varah of the University of British Columbia provided helpful discussions on the numerical methods used in Chapters III and V, and his seminar on numerical stability of finite difference methods was the stimulus for the nonlinear numerical stability results in Chapter V.

John Ahner of Vanderbilt University and Marc Mangel, now of the Operations Evaluation Group at the Center for Naval Analyses, have given constant encouragement during the preparation of this thesis.

Henry Tuckwell, now at the Department of Biomathematics of the University of California at Los Angeles, helped in many ways. I became interested in Stein's model from his discussion of it in a seminar on mathematical models in neurophysiology. Our paper solving the associated first passage time problem was my first publication. His generous and enthusiastic interest was a great stimulus during the research for this thesis.

Phil DePoy, Frank Schwamb, and Mike McCrea of the Operations Evaluation Group at the Center for Naval Analyses provided pleasant circumstances for the final writing of this thesis. Suzi Suttle and Terry Story, with the assistance of Anita Coffey, all from CNA, have skillfully prepared the manuscript.

And my wife, Debbie, has maintained infinite consideration and good humor through this lengthy process.

TABLE OF CONTENTS

TABLE OF CONTENTS
(Continued)

CHAPTER I

INTRODUCTION TO REACTION--DIFFUSION EQUATIONS

Motivation for the Study of Reaction-Diffusion Equations

This thesis studies certain problems connected with reaction-diffusion equations which are systems of partial differential equations of the form

$$\underset{\sim}{u}_t = \underset{\sim}{F}(\underset{\sim}{u}) + K\nabla^2 \underset{\sim}{u}, \tag{1.1}$$

where $\underset{\sim}{u}$ is an N-dimensional vector, K is a nonnegative-definite diffusion matrix, and $\underset{\sim}{F}(\underset{\sim}{u})$ is a vector reaction function. It will usually be assumed that K is diagonal, which is usually the case in application (but not always, see the Keller and Segel work described later in this section). If K is positive-definite, of course, a linear transformaion of $\underset{\sim}{u}$ exists such that the diffusion matrix in the new variables is diagonal. The kinetic equations of (1.1) are the equations without the spatial terms:

$$\underset{\sim}{u}_t = \underset{\sim}{F}(\underset{\sim}{u}). \tag{1.2}$$

The kinetic system (1.2) will generally be assumed to possess a stable limit cycle solution $\underset{\sim}{U}(t)$ with period T, which is then a solution of (1.1) also. This thesis is basically a study of the limit cycle as a solution of (1.1) with related results arising in the course of the study.

The first three sections of this chapter are introductory. The first section is a discussion of results from biology and chemistry involving kinetic processes or diffusion processes or both. This section concerns both experimental work and mathematical models. Although its main purpose is to provide background for the thesis research, I have included material at the end which is not related to the research here but which rounds off the discussion.

The second section discusses three papers on the mathematics of reaction-diffusion systems, which I consider classics for their combination of breadth and rigor. This section goes into more detail mathematically than the first. In these two sections, points arise which have been pursued in this thesis and these points are mentioned as they occur. The third section is a summary of the thesis itself.

The fourth section begins the thesis research proper with the study of certain reaction-diffusion equations processing explicit solutions. The study of these equations illustrates the various types of behavior which can occur as well as ideas from the papers of the second section.

Systems of the form (1.2) arise in chemistry and in population dynamics. In population dynamics, $\underset{\sim}{u}$ represents a vector of populations, e.g., of predator and prey. Both actual populations and solutions of proposed model equations exhibit rich dynamical behavior, e.g., periodic oscillations. For example, Solomon (1969) mentions oscillations with a period of 30-40 days in laboratory populations of the Australian sheep blowfly raised under limited food supplies (a small number of flies lays many eggs, the resulting population exceeds the food supply, reduces to a small population, which in turn lays many eggs, etc.), and also gives examples of laboratory prey-predator systems showing oscillations (predators eat almost all the prey, the predators die off, the prey builds up because there is almost no predation, then the predators increase, etc.). One of the earliest attempts to give a mathematical model of periodic oscillations in a prey-predator system is the Lotka-Volterra model (Lotka, 1956, Chapter 8)

$$\frac{du}{dt} = ru - \alpha uv,$$

$$\frac{dv}{dt} = -dv + \beta uv, \quad r, d, \alpha, \beta > 0. \tag{1.3}$$

Here u and v correspond to the prey and predator populations, respectively, and the uv-terms represent a decrease (increase) in prey (predator) population resulting from their random meetings. The system (1.3) is integrable and has a 1-parameter family of periodic solutions. However, this is too much of a good thing--the random effects of any biological environment would cause the population to wander from one period solution to another. The oscillations observed in practice, however, are more or less fixed and resemble stable limit cycles, since such dynamics would keep pushing a population, continually disturbed by noise, back to a fixed period solution. Bazykin (1975) gives a hierarchy of successively more complicated model equations, involving reasonable assumptions on prey-predator interactions, many of which show stable limit cycles as well as stable critical points.

In chemistry (1.2) represents the kinetic equations for a chemical system. The vector $\underset{\sim}{u}$ gives concentrations of various chemical species and $\underset{\sim}{F}(\underset{\sim}{u})$, generally nonlinear, is determined from the chemical reactions by the law of mass action. As a simple example of this law, if the chemical radicals A,B unite to form C according to

$$mA + nB \rightleftharpoons C,$$

then the associated kinetic equations, where a,b,c represent mole-concentrations of A,B,C, are

$$\begin{aligned}
\frac{da}{dt} &= -k_1\, a^m b^n + k_2\, c, \\
\frac{db}{dt} &= -k_3\, a^m b^n + k_4\, c, \qquad (1.4) \\
\frac{dc}{dt} &= k_5\, a^m b^n - k_6\, c,
\end{aligned}$$

the rate constants $k_1, \ldots, k_6$ are empirical but various relations exist between them (for instance, at equilibrium, $a^m b^n/c = k = k_2/k_1 = k_4/k_3 = k_6/k_5$; also see Fermi, 1956, Chapter 6 for the classic thermodynamical derivation of the dependence of the k_i on temperature).

(Lotka was very heavily influenced by ideas and methods of physical chemistry in his approach to biological systems. Tyson and Light (1973) note that (1.3), aside from being used as a population model, was also presented by Lotka in 1920 as the kinetics for the hypothetical chemical system

$$\begin{aligned} A + U &\to 2U, \\ U + V &\to 2V, \\ V &\to \end{aligned} \tag{1.5}$$

Note that these kinetics differ from those leading to (1.4) in that there are no back reactions. In (1.3) u,v correspond to mole concentrations of U,V. In the first reaction, A is assumed to be a substance in great excess, hence of essentially constant concentration, and the reaction, in which the presence of U stimulates the production of more U, is termed <u>autocatalytic</u>.)

Prigogine and Lefever (1968) proposed a simple model for a hypothetical chemical system with a stable limit cycle solution. The reactions for this model are (the k_i are rate constants):

$$\begin{aligned} A &\to U, && (k_1) \\ 2U + V &\to 3U, && (k_2) \\ B + U &\to V + D, && (k_3) \\ U &\to E && (k_4). \end{aligned} \tag{1.6}$$

If $\hat{a},\hat{b},\hat{u},\hat{v}$ are mole concentrations of A,B,U,V and the substances A,B are present in such large quantity as to stay essentially constant in concentration, then the kinetic equations corresponding to (1.6) are

$$\frac{d\hat{u}}{dt} = k_1 \hat{a} - k_3 \hat{b} \hat{u} - k_4 \hat{u} + k_2 \hat{u}^2 \hat{v},$$
$$\frac{d\hat{v}}{dt} = k_3 \hat{b} \hat{u} - k_2 \hat{u}^2 \hat{v}. \tag{1.7}$$

Appropriate rescaling of $\hat{a},\hat{b}$, $\hat{u},\hat{v},t$ to a,b, u,v,t reduces the number of parameters, yielding the system known as the <u>Brusselator</u> for its place of origin:

$$\frac{du}{dt} = a - (b+1)u + u^2v,$$
$$\frac{dv}{dt} = bu - u^2v. \tag{1.8}$$

Although Prigogine and Lefever (1968) note that the trimolecular autocatalysis (second reaction in (1.6)) may be physically unrealistic (and in fact no actual chemical example is known for these kinetics), the reactions are still possible and the system is one of the simplest mathematical models yielding limit cycle solutions. The unique critical point is at $u = a$, $v = b/a$ and this point becomes unstable for $b > a^2 + 1$, yielding a stable limit cycle by a Hopf bifurcation. The system has been intensively studied: numerical calculations and a rough asymptotic study are done in Lavenda, Nicolis, and Hershkowitz-Kaufman (1971), an asymptotic expression for the limit cycle period as $b \to +\infty$ is obtained in Boa (1976), and Tyson and Light (1973) show -- assuming a 2-component chemical system with at most trimolecular reactions -- that stable limit cycles apparently can occur only for reactions involving an autocatalytic step of the form $2U + V \rightarrow 3U$ and that the resulting kinetic equations are all very similar to the system (1.7).

Interest in chemical oscillations increased when Belousov (1958) discovered a fairly simple mixture (malonic and sulfuric acids, bromate and cerous ions, with the indicator ferroin) that oscillates in color with a period of about half a minute; if kept stirred, the oscillations will go on for hours. (Spatial changes discovered by Zaikin and Zhabotinskii (1970) are discussed below.) Although the full series of reactions involved is quite complicated, apparently involving 11 substances (Noyes, Field, and Körös, 1972a,b), a model based on 3 major components (Field and Noyes, 1974) yields a limit cycle solution. The reaction can be studied quantitatively in considerable detail using electrodes sensitive to specific ions--see Noyes, Field, and Körös (1972a) or, for graphs of concentration vs. time without a description of the experimental method, see Kasparek and Bruice (1971). The existence of periodic solutions for the three-dimensional Field-Noyes model was proven by Hastings and Murray (1975). Their proof is an excellent example of a useful idea from the qualitative theory of differential equations. They began by constructing a box with the three-dimensional flow of the system entering every side, so that solutions necessarily remained bounded, and containing a single critical point r_0 with one real negative eigenvalue and two complex eigenvalues with positive real parts. They then split the box into 8 sub-boxes, centered at r_0, and showed that once an orbit entered one of a chain of 6 boxes, it remained in and cycled through those 6 boxes. Finally, to show the circuit of 6 boxes contained a limit cycle, they found a portion of the surface of one box was mapped into itself by the Poincaré map (sending a point in the surface to its image point in the surface under the kinetic flow). This gives a continuous mapping of a portion of the plane into itself and the Brouwer Fixed Point Theorem implies a fixed point. The solution corresponding to a fixed point under the Poincaré map is the limit cycle.

In addition to this oscillatory inorganic reaction, a number of organic oscillatory reactions are known (three examples with model equations are mentioned in Prigogine, Lefever, Goldbeter, and Herschkowitz-Kaufman (1969)). Of particular interest here is the case of the synchronous fireflies (Buck and Buck (1976)). Certain fireflies of the Far East (especially Thailand and Borneo) flash their lights periodically with great regularity (period of .560 seconds at ambient temperature of 25° C.). If a stimulus light--flashing at a different frequency than the firefly--is applied to the firefly, the firefly's frequency changes to that of the stimulus <u>but</u> with a precisely defined phase shift. Furthermore, a treeful of these fireflies, initially flashing at random, will gradually synchronize so that the whole tree flashes on and off twice a second. Some rough modeling has been done on this phenomenon (although the underlying reactions are unknown) and there seems plenty of room for further study.

Winfree (1974) has discussed a very interesting way of using the presence of a stable limit cycle to investigate the state space of a kinetic system. Let $\underset{\sim}{U}(t)$ be the stable limit cycle in R^n with period T and $\underset{\sim}{U}(0)$ be specified, so the limit cycle is uniquely determined. If a point P close to the limit cycle is the initial point of a trajectory, then as $t \to +\infty$, the trajectory $\sim \underset{\sim}{U}(t+\phi)$ for some ϕ, $0 \leq \phi \leq T$. The constant ϕ is the <u>asymptotic phase</u> of P. For a given ϕ, one expects an (N-1)-dimensional surface, consisting of all points with the same asymptotic phase ϕ and crossing the limit cycle at $\underset{\sim}{U}(\phi)$, to exist; these surfaces are called <u>isochrons</u> by Winfree. Notice the experimental simplicity of the isochron structure: for each initial point, simply measure one number, the asymptotic phase. Winfree (1974) mentions several experiments in which the idea has been used (although the experiments have generally involved mixtures of cells, hence introducing diffusion across cell walls and complicating the results). He also explores certain experimental consequences of the existence of isochrons. Asymptotic phase is an old idea in the theory of differential equations, but results concerning it are more along the lines of existence theorems than practical computational methods. Winfree (1978) proposed the computation of isochrons (or asymptotic phase) as a research problem, and this problem is studied in Chapter III.

Having discussed the origin of kinetic systems (1.2) in population dynamics and chemistry and the importance of stable critical points and limit cycles in physical situations, we now consider systems involving kinetics plus diffusion (1.1). Diffusion arises here because of the tendancy of a high concentration (whether of ions or animals) to spread into areas of low concentration.

We shall first consider the effects of diffusion on the stationary states of (1.1), which are just the stationary states of the kinetic system. Turing (1952) was the first to recognize the importance of including the diffusion terms with the kinetic equations. Naively, one expects the addition of diffusion to a system to dampen solutions, hence increasing the stability of any stationary states. Turing showed, however, that a stationary state, stable as a solution of the kinetic system, could become linearly unstable as a solution of the reaction-diffusion system (see the next section for examples). The diffusion-induced instability became the basis of Turing's diffusion model of pattern formation in biological organisms. Roughly speaking, Turing proposed the existence of morphogens, substances inducing growth, which would tend to concentrate themselves in certain areas and cause developmental growth in those areas. His key point is that chemical kinetics coupled with diffusion is sufficient to explain the existence of discrete areas of concentration. For example, a morphogen (or activator of growth) might be chemically changed by another substance (an inhibitor, since it destroys the growth stimulating morphogen). From kinetics alone, the two substances would tend to a steady state. However, diffusion may act to destabilize that steady state, leading to -- for example -- alternating patches of high inhibitor and high activator concentrations, i.e., alternating patches of no growth and growth.

Turing advanced his model as a theory and did not attempt any analysis of actual cases, although he did mention a number of relatively simple biological examples which strongly suggested the sort of instability he proposed. For example, the Hydra is a tiny, transparent, sacklike creature whose mouth -- the mouth of the sack -- is fringed with tentacles. For simplicity, Turing had solved his equations on the circle. Applying separation of variables to his linearized equations gave him an infinite set of periodic eigenfunctions, a finite subset of which could be unstable. An unstable eigenfunction would lead to alternating patches of tentacle-producing morphogen with inhibitor between, hence the Hydra's tentacles.

The aggregation of slime mold amoebae and the creation of poly-clones in the imaginal disc of Drosophila melanogaster provide two remarkable examples of Turing's theory of morphogensis.

In the absence of food (bacteria), slim mold amoebae first tend to spread into a homogeneous layer over a surface and then begin aggregation at a number of points (called "centers"). At each center the resulting clump of cells forms into a multicellular fruiting body, generating spores. It is known that aggregation is mediated by acrasin: amoebae follow increasing concentrations of acrasin. Keller and Segel (1970) proposed a reaction-diffusion model for the aggregation of the amoebae. Briefly, the simplified form of the model consists of two components, amoebae density and acrasin density, and aggregation occurs when the stationary state becomes unstable. The model predicts qualitatively what is observed and, since all quantities are experimentally measurable, quantitative comparison is possible. Interestingly, the diffusion matrix is nondiagonal. Since the amoebae are assumed to move away from high concentrations of amoebae and towards high concentrations of acrasin, the flow of amoebae is a linear combination of the gradients of amoebae and acrasin, leading to $\frac{\partial a}{\partial t} = \nabla(D_2 \nabla a - D_1 \nabla \rho)$ where a = amoebae density and ρ = acrasin density.

The concept of polyclones requires some explanation. The following description is based on Garcia-Bellido, Lawrence, and Morata (1979), Crick and Lawrence (1975), and Kaufmann, Shymko, and Trabert (1979). The egg of the fruit fly Drosophila melanogaster hatches, the animal goes through three larval stages, and then becomes the adult. The adult is formed from the histoblast and the imaginal discs, collections of cells which remain intact during the larval stages and which take little part in laval development. There are 19 imaginal discs — 9 pairs and a single genital disc. Each pair generates a certain part of the fly, the left and right members of the disc forming the left and right members of that part. The wing disc, for instance, is associated with the wings; the left wing disc produces the left wing and a portion of the thorax at its base. It is estimated that only 15-30 cells form the wing disc at the beginning fo the first larval stage; these cells increase to about 50,000 in the wing disc at metamorphosis.

If a cell from the left wing disc is picked at some point before metamorphosis, then the descendents of that cell form a patch on the left wing. If the cell is chosen early, the eventual patch is large because there is time for the cell to have many descendents; if the cell is chosen late, the patch is small. Ingenious experiments have shown that, at a certain point in the growth of the left wing disc, a boundary line has formed so that cells on one side yield patches at the front of the wing and cells on the other yield patches at the rear of the wing. There is a well-defined boundary line, the same in all wings, separating the patches. This boundary line separates the wing into 2 halves, called compartments. The cells of one compartment form a polyclone, a group of cells comprising all descendants of some original group of a few cells (just as a clone consists of all the descendents of a single cell).

In short, at a certain stage in its development, the left wing disc has 2 compartments formed within it. One compartment becomes the front of the wing, the other the rear. (It should be emphasized that the boundary is an invisible one and can only be inferred by determining in which part of the wing the descendents of a given cell lie.) As the wing disc grows, further boundary lines -- separating top from bottom of the wing, etc. -- form. Figure 1a shows a sketch of the development of 5 compartments in the left wing disc. Again, the boundaries of these compartments are invisible -- there is no mechanical basis for the separation.

It might seem necessary at first glance to assume a different chemical basis for each boundary line formed. However, Kaufman, Shymko, and Trabert (1978) have proposed a model explaining the successive appearance of the boundaries and giving their approximate shape using a single 2-component reaction-diffusion system.

To illustrate their idea, consider a scalar diffusion equation with no-flux boundary conditions on an interval of length ℓ:

$$u_t = u_{xx} + u - u^3,\ 0 \le x \le \ell,\ u_x(0,t) = u_x(\ell,t) = 0. \tag{1.8}$$

All solutions will be bounded in time by the $-u^3$ term. The linearized equation about the stationary state $u = 0$ is

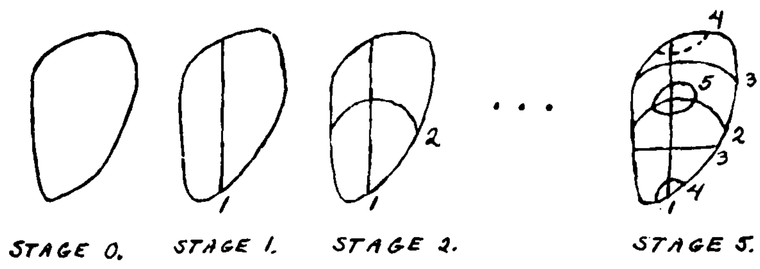


FIGURE 1A. SKETCH OF 5 SUCCESSIVE STAGES OF DEVELOPMENT IN LEFT WING DISC, BASED ON KAUFMAN, SHYMKO, TRABERT (1978). (THE DOTTED LINE 4 IS PREDICTED BUT NOT YET EXPERIMENTALLY OBSERVED.)

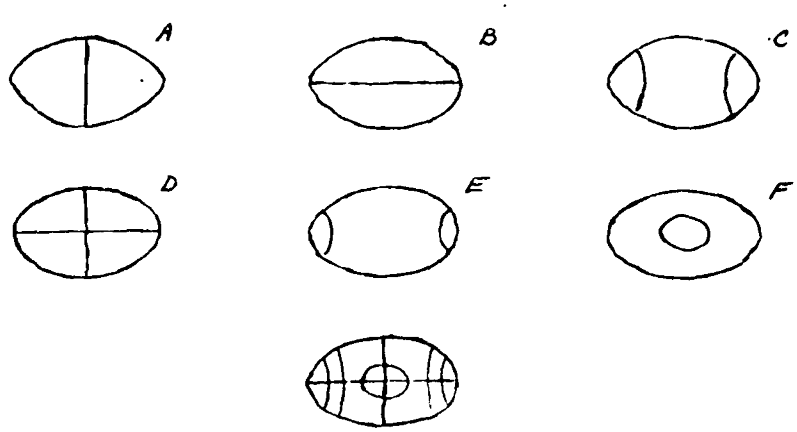


FIGURE 1B. NODAL LINES OF THE FIRST 6 EIGENFUNCTIONS OF A LINEARIZED 2-COMPONENT REACTION-DIFFUSION SYSTEM, WITH THEIR SUPERPOSITION, FROM KAUFMAN, SHYMKO, TRABERT (1978).

$$w_t = w_{xx} + w \quad \text{with solutions} \quad w_n = \exp(\lambda_n t)\cos\left(\frac{n\pi}{\ell}x\right)$$

$$\lambda_n = 1 - \left(\frac{n\pi}{\ell}\right)^2 \quad , \; n = 0,1,2,\ldots \; . \tag{1.9}$$

If ℓ is small, only the "wave number" $n=0$ is unstable; but as increases, more values of n become unstable. These unstable solutions of linearized equations can be expected to grow into stable, bounded, spatially inhomogeneous, steady-state solutions of (1.8). In other words, as the interval grows larger, (1.8) can be expected to pick up new stable steady-state solutions, referred to as stable eigenfunctions of (1.8).

In the same way, as the wing disc grows, stable eigenfunctions of a hypothetical 2-component system are expected to arise, and their nodal lines are assumed to furnish the boundaries of the compartments. Kaufman, Shymko, and Trabert did calculations to find the eigenfunctions and their nodal lines for the (linearized) 2-component system on an ellipse, which should approximate the nodal lines of the nonlinear eigenfunctions. The sequence of nodal lines for the first 6 eigenfunctions is given in Figure 1b; the superposition of the nodal lines is also given -- note the remarkable resemblance to the actual wing disc!

Incidentally, Kaufman, Shymko, and Trabert used the ellipse as an approximation to the (left) wing disc because it was the most complicated geometry for which the (linearized) equations could be solved exactly. Another reason for using the ellipse instead of the mathematically simpler circle has been mentioned by Hiernaux and Erneux (1979): in going from the circle to the ellipse, symmetry lessens and a richer family of eigenfunctions and nodal line patterns appears.

We now move on to further remarkable behavior in connection with the Belousov-Zhabotinskii reaction. Zaikin and Zhabotinskii (1970) reported that when the Belousov reagent is observed in a thin layer ($\sim$1-1/2 mm) concentric outward-moving bands of color appear. Specifically, let the Belousov reagent be chosen so that the color oscillations are between blue and red. If the red mixture is poured into a thin layer, it will spontaneously develop small blue spots which grow, each of which then develops a red spot at its center, which grows and develops a central blue spot, etc., eventually forming an expanding series of red and blue rings, or <u>target patterns</u>, in Howard and Kopell's terminology. Winfree (1972, 1974) discovered the existence of <u>spiral waves</u> spontaneously generated by the Belousov-Zhabotinskii reagent and demonstrated that the initiation of the patterns was due to dust on the surface of the solution or irregularities on the surface of the container.

The basic question in these pattern developments concerns the mechanism by which the patterns sustain themselves. Does the interaction of chemical kinetics and diffusion alone suffice for an explanation, or is some further mechanism at work? Kopell and Howard (1973) made the first rigorous investigation of this problem. Since the wave fronts for both circular and spiral waves are almost parallel at large distances from the center of the pattern, they considered the question of the existence of periodic traveling wave solutions (wave fronts exactly parallel), that is, solutions of the form $U(bt - \underset{\sim}{k}\cdot\underset{\sim}{x})$, to (1.1). The kinetic equations of (1.1) were assumed to have an unstable (spiral) critical point and a stable limit cycle. They found that traveling waves could arise as perturbations of the critical point--these could be shown to be linearly unstable as solutions of (1.1). They also found traveling waves arising as perturbations from the limit cycle—stability in general could not be shown for these, but linear stability in a special class of cases could be shown. Their results indicated circular and spiral waves arose from the limit cycle solution. Many suggestive calculations to show the existence of circular and spiral waves have been done (Ortoleva and Ross, 1974; Kuramoto and Yamada, 1976; Yamada and Kuramoto, 1976). Greenberg (by formal calculations in (1976) and with a rigorous proof in (1978)) proved the existance of circular waves for reaction-diffusion equations. Cohen, Neu, and Rosales (1978) gave a rigorous proof of the existence of spiral waves for reaction-diffusion equations. In both these proofs the circular and spiral waves were constructed from the limit cycle solution, showing it to be the source (modified by diffusion) of these remarkable waves, that is, the kinetics and diffusion alone suffice to explain their existence.

In this section we have considered--from both the physical and the theoretical sides--a hierarchy of situations. Kinetics alone give equations of the form (1.2); the main solutions are the stable critical points and the stable limit cycles. When diffusion terms are added (as Turing showed they should be) to form (1.1), the stable critical points and stable limit cycles give rise to new types of solutions, which appear to be adequate to reproduce the pattern formations observed in biological and chemical systems. It should be emphasized that few of the systems which have been mathematically studied are claimed to be models of a specific biologial or chemical system.

Before continuing with the more detailed discussion in the next section, I would like to round off this discussion of reaction-diffusion equations by mentioning other types of "simple" solutions, namely, fronts and pulses.

Traveling waves in general for (1.1) are bounded solutions of the form $\underset{\sim}{U}(\xi)$, $\xi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x}$, which converts (1.1) into a system of ordinary differential equations (ODEs) of order 2N:

$$\underset{\sim}{U}' = \underset{\sim}{F}(\underset{\sim}{U}) + K\underset{\sim}{U}''. \tag{1.10}$$

Periodic waves with $\underset{\sim}{U}(\xi)$ periodic have already been discussed. Two other important types of waves occur when $\lim_{\xi\to\pm\infty} \underset{\sim}{U}(\xi)$ exist: <u>fronts</u>, when $\underset{\sim}{U}(-\infty) \neq \underset{\sim}{U}(+\infty)$, and <u>pulses</u>, when $\underset{\sim}{U}(-\infty) = \underset{\sim}{U}(+\infty)$. Note that for these wave solutions to exist, $\underset{\sim}{U}(\pm\infty)$ must be critical points in the 2N-dimensional phase space for (1.10). A trajectory connecting two different critical points is called <u>heteroclinic</u> and a trajectory which leaves from and returns to the same critical point is called <u>homoclinic</u>.

The equation

$$u_t = u_{xx} + f(u), \quad f(0) = f(1) = 0, \quad f(u) > 0 \text{ and concave on } (0,1),$$
$$f'(0) = \alpha > 0, \quad f'(1) = -\beta \leq 0, \tag{1.11}$$

occurs in a simple model for the spread of favorable genes and was studied by Kolmogorov, Petrovsky, and Piskunov (KPP) in 1937. Their work is discussed in Sattinger (1976). They showed (1.11) possesses a traveling front solution, $U(\xi)$, $\xi = x + ct$, $U(-\infty) = 0$, $U(+\infty) = 1$, $U(\xi)$ monotone, for $c \geq 2/\alpha^{1/2}$, and obtained some stability results for these wave solutions.

Huxley's equation,

$$u_t = u_{xx} + u(1-u)(u-a) \tag{1.12}$$

has traveling fronts given exactly by $U(\xi) = 1/(1 + \exp(-\xi/2^{1/2}))$, $c = 2^{1/2}(\frac{1}{2} - a)$. It arises in connection with the FitzHugh-Nagumo equations discussed below; Fife and McLeod (1975) obtained stability results for these waves.

In 1952 (the same year as Turing's paper) Hodgkin and Huxley published a quantitative theory of the action potential for the squid giant axon. Roughly speaking, the external parts of the nerve cell are the cell body, small short fibers called dendrites, and an especially long fiber called the axon. At rest, the nerve cell maintains a certain negative potential across its cell membrane, negative inside relative to the outside. Small inputs of current are received over the surfaces of the dendrites and the cell body, increasing or decreasing the membrane potential (in particular, the potential at the base of the axon, called the trigger zone) until a threshold value is crossed, at which time an action potential--a sharp spike of high positive potential--is generated at the cell body and travels down the axon.

Hodgkin and Huxley (1952) modeled the action potential in terms of 4 components governed by a system of equations of the form:

$$\begin{aligned} V_t &= V_{xx} + f(V,\underset{\sim}{W}) \\ \underset{\sim}{W}_t &= \quad \underset{\sim}{g}(V,\underset{\sim}{W}), \end{aligned} \tag{1.13}$$

where $V(x,t)$ is the membrane potential and $\underset{\sim}{W}$ is a 3-component vector for quantities determining the conductance of the membrane to sodium and potassium ions. The components of W are identified with "potassium activation, sodium activiation, and sodium inactivation" (the physical mechanisms governing them are currently under study by numerous investigators). Hodgkin and Huxley were able to determine experimentally the forms of f and $\underset{\sim}{g}$ and, integrating the equations on a desk calculator, obtained pulse solutions corresponding to the action potential. They received the 1963 Nobel Prize for their work.

The 4 variables of the Hodgkin-Huxley system make it extremely difficult to investigate mathematically. FitzHugh (1961) derived a 2-component model for the kinetic part of the Hodgkin-Huxley equations, and Nagumo, Arimoto, and Yoshizawa (1962) added spatial terms and devised an electrical circuit as a representation of the system (the representation was possible because the nonlinear part of the 2-component system corresponded to van der Pol's equation, which models the triode oscillator). The resulting FitzHugh-Nagumo equation is

$$\begin{aligned} u_t &= u_{xx} + u(1-u)(u-a) - v \\ v_t &= \qquad bu, \end{aligned} \tag{1.14}$$

where $b > 0$ is very small. (Huxley's equation arises from $b = 0$, $v = 0$.) Hastings (1975) and FitzHugh (1969) review work on the FitzHugh-Nagumo and Hodgkin-Huxley equations. (General surveys on reaction-diffusion systems are Cohen (1971) and Fife (1978a, 1979).)

Hastings (1974) and Carpenter (1974) have shown the existence of periodic waves to the FitzHugh-Nagumo equations; this does not follow from the general results of Kopell and Howard (1973) since the diffusion matrix is singular. Hastings (1976a), besides giving material on the periodic waves, proves the existence of pulse solutions for the FitzHugh-Nagumo equations--numerical work had indicated such pulse solutions existed. Hastings (1976b) proves the existence of pulse wave solutions to the Hodgkin-Huxley equations.

The existence of traveling fronts and pulses is far harder to show generally than the existence of periodic waves. Typically, fronts and pulses do not arise as any sort of small amplitude perturbation (in contrast to periodic waves arising by a Hopf bifurcation) nor do they arise as perturbations off some easily studied large amplitude solution (as in the case of large amplitude waves arising by perturbation off a limit cycle). To illustrate the difficulties, consider the problem of proving the existence of a front by showing the existence of a trajectory connecting two critical points in the 2N-dimensional phase space associated with (1.10). The linearization near each critical point yields the beginning and end of the trajectory, but joining the two segments requires some difficult work (assuming it is possible in the first place). Shooting methods can sometimes be used, but these are generally only for the scalar case--see the discussion of the KPP equation in Sattinger (1976). A curious aspect of fronts and pulses (the stable ones, at least) is that they can be calculated more easily by solving the full PDE system numerically than by calculating the corresponding trajectory as the solution of a system of ODEs. Initial data is almost sure to evolve to the traveling wave for the PDE solutions. However, trajectories initially close to the wave trajectory in the phase space for (1.10) usually diverge exponentially, so that extremely small numerical errors ruin the calculation. The quantitative study of fronts and pulses has been mostly numerical; a notable exception is the work by Casten, Cohen, and Lagerstrom (1975), who construct an approximation to the pulse wave for the FitzHugh-Nagumo equations. Rinzel and Keller (1973) give a very interesting approach: the nonlinear part of the FitzHugh-Nagumo is replaced by a (discontinuous) piecewise linear approximation. The traveling waves can then be found explicitly and their stability studied. This is a very powerful idea for obtaining information about the qualitative behavior of solutions and it should be used more frequently.

Evans has written a series of papers aimed towards the study of the pulse solution of the Hodgkin-Huxley equations. He studies (1.13) with $\underset{\sim}{W}$ an (N-1)-component vector. Evans and Shenk (1970) prove the existence of solutions to (1.13) using a Picard iteration argument; a boundedness result is also given, see the remarks on the Chueh, Conley, and Smoller paper in the next section. Evans (1972a) proves a stability result for the traveling wave solutions $\underset{\sim}{\phi}(x+ct)$ of (1.13). The result is especially interesting since it involves the concept of asymptotic phase for solutions of (1.13). To explain this idea, it is more convenient to use the notation of (1.1), with $K = K_o = \mathrm{diag}(1,0,\ldots,0)$, so that u_1 corresponds to V and $u_2, \ldots, u_N$ to $\underset{\sim}{W}$.

If $\underset{\sim}{u} = \underset{\sim}{\phi}(x+ct)$ is a solution of (1.1), then $\underset{\sim}{\phi}(x+ct+h)$ is also a solution for all h. Let $\underset{\sim}{\phi}(x+ct)$ be some fixed traveling wave solution and switch to moving coordinates by setting $y = x + ct$. The system (1.1) now becomes $(\underset{\sim}{v}(y,t) = \underset{\sim}{u}(x,t))$

$$\underset{\sim}{v}_t + c\underset{\sim}{v}_y = \underset{\sim}{F}(\underset{\sim}{v}) + K_o\underset{\sim}{v}_{yy} \tag{1.15a}$$

with the solutions $\underset{\sim}{\phi}(y+h) = \underset{\sim}{v}$. Now the most that can be expected so far as stability is concerned is that initial data of the form $\underset{\sim}{\phi}(y) + \epsilon\underset{\sim}{f}(y)$, ϵ small, will evolve to $\underset{\sim}{\phi}(y+\epsilon h)$ as $t \to +\infty$ in (1.15a), where ϵh is the <u>asymptotic phase</u> resulting from $\epsilon\underset{\sim}{f}(y)$. Furthermore, the linearized system about $\underset{\sim}{\phi}(y)$ obtained by setting $\underset{\sim}{v}(y,t) = \underset{\sim}{\phi}(y) + \underset{\sim}{w}(y,t)$ in (1.15a) and dropping nonlinear terms is

$$\underset{\sim}{w}_t + c\underset{\sim}{w}_y = \nabla\underset{\sim}{F}\,(\underset{\sim}{\phi}(y))\,\underset{\sim}{w} + K_o\underset{\sim}{w}_{yy}, \tag{1.15b}$$

which has $\underset{\sim}{\phi}'(y)$ as a solution, corresponding to a 0-eigenvalue of this linear operator. Thus, even if the remaining spectrum has negative real part, initial data $\underset{\sim}{w}(y,o)$ will not decay to 0, but to some $\hat{h}\,\underset{\sim}{\phi}'(y)$.

Consequently, Evans is forced to define stability in the following way. The linearized system (1.15b) is <u>exponentially stable at $\underset{\sim}{\phi}'$</u> if solutions decay expoentially to $\hat{h}\underset{\sim}{\phi}'(y)$ for some constant $\hat{h}$, and the full system (1.15a) is <u>exponentially stable at $\underset{\sim}{\phi}$</u> if initial data $\underset{\sim}{\phi}(y) + \epsilon \underset{\sim}{f}(y)$ decays exponentially fast to $\underset{\sim}{\phi}(y+\epsilon h)$ for some h. Evans' main theorem is that (1.15a) is exponentially stable at $\underset{\sim}{\phi}$ if (1.15b) is exponentially stable at $\underset{\sim}{\phi}'$, i.e., the linearized system determines the stability of the nonlinear system. A constant solution is trivially a traveling wave and Evans (1972b) applies the stability result to constant solutions of (1.13), since the linearized system has constant coefficients and is relatively easy to study. Evans (1972c) returns to the full traveling wave and considers the linearized system further, investigating ways of calculating the spectrum. Evans and Feroe (1977?) apply the results of (1972c) to numerical calculations for traveling waves in the actual Hodgkin-Huxley equations.

Sattinger (1976) proves results analogous to Evans for other systems of the form (1.1). Roughly speaking, for systems (1.1) with K a positive-definite diagonal matrix and possessing traveling waves $\underset{\sim}{u} = \underset{\sim}{\phi}(x+ct)$, Sattinger shows that if the spectrum of the linearized system (except for the eigenvalue 0 resulting from the solution $\underset{\sim}{\phi}'$) lies in the left-half-plane and can be bounded strictly away from the imaginary axis by a parabola $x = -ay^2 + b$, $a,b > 0$, then in the full system (1.1) initial data of the form $\underset{\sim}{\phi}(y)+\epsilon\underset{\sim}{f}(y)$ $(y = x + ct)$ converges exponentially to $\underset{\sim}{\phi}(y+\epsilon h)$ for some constant h.

A second aspect of Sattinger's work of importance equal to his stability result is his introduction of weighted sup norms (both Evans and Sattinger use sup norms for their stability results), for instance,

$$||u(y)|| = \sup_{-\infty < y < +\infty} |\exp(cy)\, u(y)| .$$

The basic reason for introducing such a new norm is that the hypotheses of the stability theorem may not apply if the usual sup norm is used because it may not be possible to bound the spectrum away from the imaginary axis; the spectrum is shifted under the weighted norm and the hypotheses may then apply. The weight function is chosen to relate solutions of the linearized system to the adjoint system to help in calculating the spectrum (Sattinger, 1977).

Basic Ideas Illustrated by Three Classic Papers

The purpose of this section is to study three classic papers on reaction-diffusion equations by discussing their content, illustrating their content by explicit calculations, and discussing related work. In approaching the very broad class of partial differential equations represented by (1.1), it is useful to keep some basic questions in mind to aid in fitting together pieces of results from different papers. I shall mention three such basic questions and then proceed with the detailed discussion of the papers.

Question 1. Do "simple" solutions of (1.1) exist?

"Simple" here means possessing "notable" qualitative features and does not refer to ease of calculation. Examples of what we mean by simple solutions are described below.

1. Stationary states of the kinetic equations (1.2) are spatially homogeneous solutions of (1.1). Limit cycle solutions of (1.2) are spatially homogeneous, time-periodic solutions of (1.1).
2. It can be shown (see Kopell and Howard below) that traveling wave solutions of (1.1) exist under fairly general conditions. These solutions are found by assuming $\underset{\sim}{u} = \underset{\sim}{u}(bt - \underset{\sim}{k} . \underset{\sim}{x})$ where b is a constant scalar and $\underset{\sim}{k}$ is a constant vector which reduces the system (1.1) to a system of ordinary differential equations. (The same assumption, of course, can lead to wave fronts or pulse solutions, or pulse trains.)
3. As mentioned in the first section, circular and spiral wave solutions can be shown to exist for certain cases of (1.1). Although more complicated than periodic waves, their construction (at least in some cases) reduces to the solution of a system of ODEs.

Notice that only solutions on the whole space (R^n) are mentioned. On a finite domain with boundary conditions the existence of simple solutions is a much more complicated problem.

Question 2. Are these simple solutions stable as solutions of (1.1)?

Basically, this question is concerned with the long-time behavior of solutions of (1.1). The experimentalist hopes that messy initial data will evolve into some well-defined easily-observed data that are close to a simple solution. A necessary condition for a simple solution to occur as the limit in the long-time behavior is stability.

Question 2 brings up the definition of stability. A precise discussion of stability involves the various types (for instance, $\underset{\sim}{u}_0(t)$ is stable if solutions initially close to $\underset{\sim}{u}_0(0)$ remain close as $t \to +\infty$; $\underset{\sim}{u}_0(t)$ is asymptotically stable if solutions initially close converge to $\underset{\sim}{u}_0(t)$; $\underset{\sim}{u}_0(t)$ is orbitally stable if solutions initially close converge to $\underset{\sim}{u}_0(t+\delta)$) in the context of spatially dependent systems, the choice of a norm (for instance, L_2 or L_∞), the problem of whether stability in one norm implies stability in another, the question of when linear stability implies "actual" stability, and so on. I shall avoid extensive discussion by simply noting that in practice stability usually means linear stability (which is still extremely difficult to handle in many cases) and that further results are available (the results of Evans (1972a,b,c) and Sattinger (1976, 1977) mentioned in the first section, of Chueh, Conley, and Smoller (1977) below).

If the simple solutions are unstable (in some sense), they cannot be candidates for the long-time behavior of the system and are usually of no further interest. (But not always! Turing's theory (Turing, 1952) of morphogenesis is based on the loss of stability of stationary states as solutions of (1.1).)

All three papers discussed here are concerned with various aspects of stability: Turing (1952) gives implications of instability, Kopell and Howard (1973) obtain two important linear stability results, and Chueh, Conley, and Smoller (1977) consider the related question of boundedness of solutions.

Question 3. If a simple solution exists and is stable (in some sense), how can its notable characteristics be calculated?

The point here is to obtain mathematical information on any properties an experimentalist may find measurable, for example, amplitude, wavelength, frequency, wave speed, asymptotic phase.

Of the three papers, only Kopell and Howard give results related to Question 3: the explicit solutions of the $\lambda-\omega$ systems and the numerical solution of an integral equation for periodic traveling waves (discussed in Chapter VI). This bias towards qualitative results is typical of the whole field of reaction-diffusion equations because the rich qualitative behavior of the systems is still being vigorously investigated and powerful methods are available for qualitative results (for example, geometric arguments for boundedness and the qualitative theory of dynamical systems for obtaining special solutions).

These three questions concerning the existence, stability, and calculation of "simple solutions" describe major activities in investigating the reaction-diffusion equations (1.1).

The papers discussed in this section are classics because they derive broad, basic results with full mathematical rigor. These papers are:

1. Turing (1952), as mentioned in the first section, shows that the addition of diffusion terms to a kinetic system may make (kinetically stable) stationary states linearly unstable.
2. Kopell and Howard (1973) prove the existence of periodic traveling waves for reaction-diffusion equations under certain conditions. One type of traveling wave arises from a

(kinetically unstable) stationary state by a Hopf bifurcation--these are shown to be linearly unstable as solutions of (1.1). The second type occurs as a type of perturbation of the kinetically stable limit cycle--there is some evidence that these are stable.

3. Chueh, Conley, and Smoller (1977) give a remarkably simple geometric criterion for showing boundedness of solutions of certain reaction-diffusion systems, leading to stability results.

Beginning with Turing's paper, consider the two-component reaction-diffusion system

$$\begin{aligned} u_t &= F(u,v) + (1+\alpha)\nabla^2 u \\ v_t &= G(u,v) + (1-\alpha)\nabla^2 v, \qquad |\alpha| \le 1. \end{aligned} \tag{2.1}$$

(Any two-component system (1.1) can be placed in this form by rescaling the space variables.) Let $(u,v) = (0,0)$ be a stationary state of the system and linearize about this solution. Keeping the same letters u,v for the dependent variable in the linearized system, it can be written as

$$\begin{aligned} u_t &= Au + Bv + (1+\alpha)\nabla^2 u \\ v_t &= Cu + Dv + (1-\alpha)\nabla^2 v, \qquad |\alpha| \le 1, \end{aligned} \tag{2.2}$$

where $A = F_u(0,0)$, etc., define the constants A,B,C,D. Separating variables by setting $(u,v) = (\hat{u}(t)\exp(-i\underset{\sim}{k}\cdot\underset{\sim}{x}),\ \hat{v}(t)\exp(-i\underset{\sim}{k}\cdot\underset{\sim}{x}))$ (equivalently, Fourier transforming) yields the system

$$
\begin{aligned}
\hat{u}_t &= A\hat{u} + B\hat{v} - (1+\alpha)k^2\hat{u} \\
\hat{v}_t &= C\hat{u} + D\hat{v} - (1-\alpha)k^2\hat{v}, \qquad |\alpha| \leq 1.
\end{aligned}
\tag{2.3}
$$

The general solution of (2.3) has the form $(\hat{u},\hat{v}) = (\hat{u}_0 \exp(+\lambda t),\ \hat{v}_0 \exp(+\lambda t))$, where λ satisfies the characteristic equation

$$
\begin{aligned}
\lambda^2 - (A + D - 2k^2)\lambda + (AD - BC - ((1-\alpha)A + (1+\alpha)D)k^2 \\
+ (1-\alpha^2)k^4) = 0.
\end{aligned}
\tag{2.4}
$$

The stationary state is linearly unstable as a solution of (2.1) if the characteristic equation has roots λ with positive real part. Turing assumes the stationary state is stable as a solution of the kinetic system (that is, when $k^2 = 0$):

$$
\begin{aligned}
A + D &\leq 0 \quad \text{(the sum of the roots is nonnegative)} \\
AD - BC &\geq 0 \quad \text{(the product of roots is nonnegative)}
\end{aligned}
\tag{2.5}
$$

Since $A + D - 2k^2 < 0$ for $k^2 > 0$ follows from (2.5), the sum of the characteristic roots in (2.4) is always negative for $k^2 > 0$. However, the product need not stay positive, in which case a positive characteristic root (i.e., instability) occurs.

Specifically, positive roots of (2.4) occur for

$$|\alpha| = +1 \text{ (singular diffusion matrix)}, \ (1-\alpha)A + (1+\alpha)D = E_1 > 0 \ \text{ and } \ k^2 > (AD - BC)/E_1; \tag{2.6a}$$

$$|\alpha| < 1 \text{ (nonsingular diffusion matrix)}, \ ((1-\alpha)A + (1+\alpha)D)^2 - 4(1-\alpha)^2(AD - BC) = E_2^2 > 0 \ (E_2 > 0), \text{ and} \tag{2.6b}$$
$$(E_1 - E_2)/2(1-\alpha^2) < k^2 < (E_1 + E_2)/2(1-\alpha^2).*$$

These 2 cases, dependent on the nature of the diffusion matrix, are typical in studying reaction-diffusion equations: many general results require the assumption of a nonsingular diffusion matrix, and either the proof does not carry over or the result actually does not hold in the singular case. From (2.6), for example, the (kinetically stable) stationary state is always linearly stable to perturbations with large wave number k^2 when the diffusion matrix is nonsingular; when the matrix is singular, it may be unstable for all sufficiently large k^2.

Turing (1952) used this diffusive destabilization of a steady state solution as the basis of his theory of morphogenesis, discussed in the first section. His stability results were extended by Othmer and Scriven (1969), who did a thorough study of the effects of diffusion on stationary states of all types of kinetic stability and instability. They gave a complete linearized analysis of two component systems with some results for three-component and higher dimensional systems.

*This condition can be vacuous if $E_1 + E_2 \leq 0$.

After the work of Turing (1952) and Othmer and Scriven (1969), the next natural step would be to look at the stability of limit cycle solutions of (1.1). The complication, of course, is that even for linearized stability, the resulting variational equation is a Floquet system with coefficients independent of space variables, but periodic in time. This step, however, has been passed over in the literature - although the lack of work on it has been mentioned in Kopell and Howard (1973) and Othmer (1977) - probably because attention has been focused on traveling waves and more complicated solutions. Chapter II of this thesis studies the linear stability of the (kinetically stable) limit cycle as a solution of (1.1); chapter IV discusses perturbations of the limit cycle as solutions of (1.1).

The second classic paper, Kopell and Howard (1973), was intended as a first step in studying the circular waves (or "target patterns" in Kopell and Howard's terminology) occurring in the Belousov-Zhabotinskii reaction. In their original announcement of the occurrence of circular waves, Zaikin and Zhabotinskii (1970) presented a rough model to explain the occurrence of the circular waves. The assumptions of this model, however, were rather ad hoc - for instance, points were assumed to exist in the solution at which the underlying periodic reaction proceeded with frequencies different from the bulk reaction, with no explanation of how such a difference could be maintained. Kopell and Howard wished to show that diffusion, added to the kinetics, sufficed to produce the waves. Since circular and spiral waves at great distances from their centers have almost parallel wave fronts, Kopell and Howard decided to investigate the existence of traveling wave solutions $\underset{\sim}{U}(bt - \underset{\sim}{k} \cdot \underset{\sim}{x})$ (i.e., perfectly parallel wave fronts) to (1.1).

They were aided in their studies by a remarkable set of equations, the $\lambda-\omega$ systems,

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} \lambda(R) & -\omega(R) \\ \omega(R) & \lambda(R) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} \nabla^2 u \\ \nabla^2 v \end{bmatrix}. \qquad (2.7a)$$

Using the transform $(u,v) = (R\cos\psi,\ R\sin\psi)$ yields

$$\begin{bmatrix} R_t \\ \psi_t \end{bmatrix} = \begin{bmatrix} R\,\lambda(R) \\ \omega(R) \end{bmatrix} + \begin{bmatrix} \nabla^2 R - R|\nabla\psi|^2 \\ \frac{2}{R}\nabla R\cdot\nabla\psi + \nabla^2\psi \end{bmatrix}. \qquad (2.7b)$$

Setting $\psi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x}$, $R = R_0$ constant, gives the explicit solution

$$\begin{aligned} u &= R_o \cos(bt - \underset{\sim}{k}\cdot\underset{\sim}{x}) \\ v &= R_o \sin(bt - \underset{\sim}{k}\cdot\underset{\sim}{x}) \end{aligned} \qquad \text{with} \qquad \begin{aligned} \lambda(R_o) &= k^2 \\ \omega(R_o) &= b. \end{aligned} \qquad (2.8)$$

The usual assumption on the system is $\lambda(R) > 0$ on $[0, \bar{R})$, $\lambda(\bar{R}) = 0$, and $\lambda(R) < 0$ for some range $R > \bar{R}$. Under these assumptions the kinetic equations of (2.8) have an unstable spiral point at $(u,v) = (0,0)$ and a stable limit cycle $(U,V) = (\bar{R}\cos(\bar{\omega}t),\ \bar{R}\sin(\bar{\omega}t))$ with $\bar{\omega} = \omega(\bar{R})$, and periodic traveling waves exist for all amplitudes $0 \leq R_0 \leq \bar{R}$.

For the $\lambda-\omega$ systems with their traveling waves of all amplitudes R_o, $0 \leq R_o \leq \bar{R}$, it seems equally plausible that the waves "originated" as a perturbation from the unstable stationary state or as a perturbation off the stable limit cycle. Consequently, Kopell and Howard considered the general problems of waves arising in the system (1.1), with the assumption that the kinetic equations either (a) possess an unstable spiral point (for an n-component system, a critical point with a pair of conjugate complex eigenvalues with positve real part) or (b) possess a stable limit cycle. In other words, substituting $\underset{\sim}{u} = \underset{\sim}{u}(bt - \underset{\sim}{k} \cdot \underset{\sim}{x})$ into (1.1) gives the system

$$b\underset{\sim}{u}' = \underset{\sim}{F}(\underset{\sim}{u}) + k^2 K \underset{\sim}{u}''. \tag{2.9}$$

Kopell and Howard considered whether this system possesses periodic solutions given that the kinetic system $\underset{\sim}{u}' = \underset{\sim}{F}(\underset{\sim}{u})$ has either (a) an unstable spiral point or (b) a stable limit cycle.

The Hopf Bifurcation Theorem (Hopf (1942), translated by Kopell and Howard in Marsden and McCracken (1976)) was used to prove existence of periodic traveling waves for (2.9). Roughly, the Hopf theorem says the following: Suppose a 2-component kinetic system has a stable spiral point, so all trajectories over some region in the plane flow into that point. Let the system contain a parameter and suppose that as the parameter varies, the real part of the complex conjugate eigenvalues changes from negative to positive - the critical point changes to an unstable spiral. Then, for some small range of parameter values just after the instability appears, the flow far away from the critical point remains inwardly directed because it is little affected over the small range of paramter values. Near the critical point, however, a drastic change in behavior has taken place - the ingoing flow has changed to an outgoing flow. The outgoing flow at the critical point meets the incoming flow still present in outlying regions, and a periodic solution appears where they meet. This periodic solution is the Hopf bifurcation, a periodic solution appearing when complex-conjugate eigenvalues at a critical point change their real part from negative to positive. The same geometric picture holds for multi-component systems; it is only necessary to consider the flow on the 2-dimensional manifold corresponding to the two conjugate roots.

Kopell and Howard showed that (2.9) in the 2-component case, under mild assumptions, possesses 2 pairs of complex-conjugate roots, and that for a certain relation between b and k^2, a pair of these roots crosses the imaginary axis. When this crossing takes place, the Hopf Theorem applies to give the existence of small amplitude periodic solutions to (2.9), i.e., small amplitude period traveling waves. The proof extends to the n-component case.

Kopell and Howard also showed that traveling waves originate as perturbations off the limit cycle solution. In this case, $k^2 \sim 0$ and $b \sim 1$ in (2.9), which is rewritten as an integral equation. An iterative argument, with the limit cycle $\underset{\sim}{U}$ as starting function, then constructs a periodic solution to (2.9) and a frequency $b(k^2)$, where k^2 is considered fixed.

The integral equation used by Kopell and Howard is not the most obvious choice, and I was long puzzled why they chose it. Some digging in the literature has clarified this point. Briefly, the problem they considered could be described as the persistence of periodic solutions in autonomous systems under singular perturbation (since $k^2 \sim 0$ multiplies the higher derivatives in (2.9)). Although several closely related problems (such as the case for nonautonomous systems) had been dealt with - and these will be discussed in some detail in chapter VI - the closest result appears to be a series expansion for the perturbed periodic solutions due to Wasow (1976). Wasow's series, however, is only asymptotic - he was not able to prove convergence (and, strictly speaking, did not prove the existence of the perturbed periodic solutions). In other words, Kopell and Howard's result was not merely the construction of periodic traveling waves but also a contribution to the theory of singular systems of differential equations. Their proof became all the more interesting, and a careful study of it eventually led to a second proof based on a series expansion instead of an integral equation. This series is convergent, in contrast to Wasow's asymptotic result; the essential trick is to match two powers of the small parameter instead of one and use a curious property of Floquet systems found by Kopell and Howard. The background on related problems, the construction of this series, and proof of its convergence from the subject matter of chapter VI.

Kopell and Howard showed that, in general systems of the form (2.9) as well as in λ-ω systems, small amplitude traveling waves (near the unstable stationary state) and large amplitude waves (near the limit cycle) both occurred. They next considered the linear stability of the traveling waves.

Again, λ-ω systems played an important role. The variational equation of (2.7b) around the solution $R = R_o$, $\psi = bt - \underset{\sim}{k} \cdot \underset{\sim}{x}$ with

with $b = \omega(R_o)$, $k^2 = \lambda(R_o)$ turns out to be an equation with constant coefficients. The variational equations can therefore be solved explicitly. Assuming $\lambda(R) > 0$ on $0 \leq R < \bar{R}$, $\lambda(\bar{R}) = 0$, it can be shown that the traveling wave (2.8) with amplitude R_o, $0 \leq R_o \leq \bar{R}$, is linearly stable iff

$$4\lambda(R_o)\left[\left(1 + \frac{\omega'(R_o)}{\lambda'(R_o)}\right)^2 + R_o \quad \lambda'(R_o)\right] \leq 0. \tag{2.10}$$

In particular, with $\lambda'(\bar{R}) < 0$, it follows that the waves are linearly unstable as $R_o \to 0^+$ and linearly stable as $R_o \to \bar{R}^-$, that is, small amplitude waves are unstable and large amplitude waves stable.

Kopell and Howard were actually able to show that waves of sufficiently small amplitudes arising from the unstable stationary state must be linearly unstable. The essence of their proof is to first note that the linearization of (1.1) about the stationary state has exponentially increasing solutions simply because the stationary state is kinetically unstable. The linearization of (1.1) about a wave, which itself is a small amplitude perturbation of the stationary state, leads to a linear system with coefficients which are nearly the same as those of the linearization of (1.1) about the stationary state. Consequently, the spectrum of the known unstable operator is only slightly perturbed and instability persists.

However, they were unable to obtain any general results on stability of large amplitude traveling waves. By default, it appears that these large amplitude solutions are the source of the circular and spiral waves observed experimentally.

As a sort of limiting case for traveling wave stability, Kopell and Howard briefly considered the question of whether the limit cycle solution, stable as a solution of the kinetic equations (1.2), remains stable as a solution of (1.1). They showed that if the diffusion matrix is scalar, then the limit cycle is linearly stable as a solution of (1.1) to all wave numbers k^2. No results were obtained for the non-scalar diffusion matrix case, which is a further motivation for the study of limit cycle stability in chapter II.

Howard and Kopell (1977) contains further work on traveling waves; specifically, a description of "slowly-varying" waves in which the phase $bt - \underset{\sim}{k} \cdot \underset{\sim}{x} = \theta$ is generalized to $\theta(t, \underset{\sim}{x})$ with θ_t, $\nabla\theta$ changing on very slow time- and space-scales (θ_t, $\nabla\theta$ correspond to $b, \underset{\sim}{k}$), and a discussion of "shock structures" - the small region where two traveling waves meet. Ortoleva and Ross (1973) and Kuramoto and Yamada (1976) give some formal constructions related to circular and spiral waves, but they have difficulties with singularities at the centers. Yamada and Kuramoto (1976) found spiral waves in a system whose diffusion matrix has complex eigenvalues. Greenberg (1976) gave a formal expansion for calculating circular waves which does not contain the difficulties with singularities mentioned above. Greenberg (1978) later proved that the construction was convergent for $\lambda - \omega$ systems. Cohen, Neu, and Rosales (1978) proved the existence of spiral wave solutions for λ-ω systems.

Before discussing the third classic paper in detail, it will be useful to give some perspective on the results. Chueh, Conley, and Smoller (1977) give a simple geometric criterion for boundedness of solutions of systems of reaction-diffusion equations. Basically, they show that, under certain conditions on the kinetic equations, there exist "boxes" in $\underset{\sim}{u}$-space such that any solution of (1.1) which is contained in the box at $t = 0$ remains in the box, i.e., remains bounded for all time.

Such boundedness theorems, although interesting for their own sake, do not lead directly to stability results for particular solutions--a perturbed traveling wave may transform into another wave or even a stationary state without violating the boundedness conclusion. Of course, boundedness is an important property for solutions of realistic model systems, and it can be used indirectly to obtain stability results (see reference to Conway, Hoff, and Smoller (1978) below). (Sattinger (1976) gives actual stability results for traveling wave solutions of reaction-diffusion systems; specifically, he gives conditions under which linear stability of a traveling wave implies stability with respect to the full nonlinear system.)

It is interesting to contrast the results of Chueh, Conley, and Smoller (1977) with various <u>maximum principles</u>, a traditional form of boundedness theorem. As described in Protter and Weinberger (1967), a maximum principle is a theorem to the effect that a function, satisfying some differential inequality (which may be expressed as an ODE or PDE) in a domain, has a maximum on the boundary of that domain. (A weak maximum principle asserts a maximum lies on the boundary; a strong maximum principle asserts the maximum lies <u>only</u> on the boundary, unless the function is constant.) Protter and Weinberger (1967, chapter 2) have some results for nonlinear parabolic scalar equations and parabolic systems. Chueh, Conley, and Smoller (1977) introduce fixed bounds independent of initial and/or boundary conditions.

The results of Chueh, Conley, and Smoller (1977) will be discussed in a simplified form. The reaction-diffusion system will be (1.1) with K a constant positive-definite diagonal matrix. It is assumed that:

If the initial data for (1.1) satisfies either

$$\begin{aligned} &\underset{\sim}{u}(\underset{\sim}{x},0) \to \underset{\sim}{u}_\infty, \text{ constant, as } ||x|| \to \infty, \\ \text{or} \\ &\underset{\sim}{u}(\underset{\sim}{x},0) \text{ is periodic in each component of } \underset{\sim}{x}, \end{aligned} \tag{2.11}$$

then a solution $\underset{\sim}{u}(\underset{\sim}{x},t)$ exists for some interval $0 \leq t < \delta$, and for these values of t either

$$\underset{\sim}{u}(\underset{\sim}{x},t) \to \underset{\sim}{u}_\infty \text{ as } ||x|| \to \infty$$

or

$$\underset{\sim}{u}(\underset{\sim}{x},t) \text{ is periodic in each component of } \underset{\sim}{x}.$$

Setting $\underset{\sim}{u} = (u_1, \ldots, u_N)$, $\underset{\sim}{F}(\underset{\sim}{u}) = (F_1(\underset{\sim}{u}), \ldots, F_N(\underset{\sim}{u}))$, define a "box" B by $(a_i < b_i)$

$$B = \left\{(u_1, \ldots, u_N) \mid a_i \leq u_i \leq b_i, \quad i = 1, \ldots, N\right\}. \tag{2.12}$$

Let $\underset{\sim}{n}$ be the outward unit normal to the surface of B. The kinetic equations (1.2) for (1.1) are said to define <u>flow into B</u> if $\underset{\sim}{n} \cdot \underset{\sim}{F}(\underset{\sim}{u}) < 0$ on the boundary of B. Equivalently, the kinetic flow is into B if

$F_i(u_1, \ldots, a_i, \ldots, u_N) > 0$ and $F_i(u_1, \ldots, b_i, \ldots, u_N) < 0$ on the sides of B. The following theorem is then a special case of more general results of Chueh, Conley, Smoller (1977):

THEOREM 1. If solutions of (1.1) satisfy (2.11) and if there exists a set B defined by (2.12) such that the kinetic flow is into B, then initial data $\underset{\sim}{u}(\underset{\sim}{x},0)$ satisfying (2.1i) and contained in B yields a solution $\underset{\sim}{u}(\underset{\sim}{x},t)$ that remains in B. (Since solutions initially in B remain in B for $t \geq 0$, B is referred to as a <u>positively invariant set.</u>)

The essential idea of the proof is geometric. Suppose the solution is about to escape the box across the side $u_i = b_i$. Then a maximum $u_i(\underset{\sim}{x}_o, t_o) = b_i$ will exist for some point $\underset{\sim}{x}_o$ and time t_o, with $u_i(\underset{\sim}{x},t) < b_i$ for $t < t_0$. But

$$u_{it} = F_i(u_1, \ldots, b_i, \ldots, u_N) + d_i \nabla^2 u_i$$

at the point $\underset{\sim}{x}_o$, t_o, whre $F_i < 0$ (by hypothesis) and $\nabla^2 u_i \leq 0$ (since $u_i(\underset{\sim}{x}_o, t_o)$ is a maximum). Hence $u_{it}(\underset{\sim}{x}_o, t_o) < 0$, condicting aflow out of box B.

The actual results of Chueh, Conley, and Smoller are much more general than Theorem 1 (which is adequate for all purposes of this thesis). The diffusion matrix need not be diagonal or constant; the entries may depend on $\underset{\sim}{u}$ and it is only necessary that the matrix have real, nonnegative eignevalues--in this case the positively-invariant set is to be a region bounded by surfaces normal to the ($\underset{\sim}{u}$-dependent) left-eigenvectors of K and be "quasi-convex". (In particular, if K is scalar, any quasi-convex surface will do for a boundary of the positively-invariant set!) Furthermore, first derivative terms may appear in (1.1), although this further restricts the positively invariant sets.

Chueh, Conley, and Smoller show the full set of conditions eventually derived for a positively invariant set to be a characterization: if a set is positively invariant, then it almost satisfies the above conditions. (The precise meaning "almost" can be found in their paper.) They also derive bounds on the first spatial derivative of solutions for certain reaction-diffusion systems and show how to derive bounds on the solution of certain first-order PDE's using a viscosity method (i.e., adding terms of the form $\epsilon\nabla^2 u$, deriving bounds, and letting $\epsilon \to 0$).

As an illustration of the use of a priori bounds on solutions to derive further results, a slightly simplified version of Chueh, Conley, and Smoller's result on boundedness of spatial derivatives will be given.

Consider (1.1) with

$$\underset{\sim}{u}_t = \underset{\sim}{F}(\underset{\sim}{u}) + K\,\underset{\sim}{u}_{xx},\quad \underset{\sim}{u} = (u_1, \ldots, u_N),$$

$$K = \text{diag}\,(d_1, \ldots, d_N),\quad d_i > 0; \tag{2.13a}$$

$$\underset{\sim}{u}(x,0) \text{ satisfies periodic B.C. on } 0 \leq x \leq L; \tag{2.13b}$$

there exist constants m_i, $\hat{m}_i$ such that

$$m_i \leq u_i\,(x,0) \leq \hat{m}_i,\quad i = 1, \ldots, N \text{ imply}$$

$$m_i \leq u_i(x,t) \leq \hat{m}_i,\quad i = 1, \ldots, N,\quad \text{for } t \geq 0. \tag{2.13c}$$

The existence of a positively invariant set for $\underset{\sim}{F}(\underset{\sim}{u})$ would, of course, be sufficient to give (2.13c). Set $\underset{\sim}{u}_x = \underset{\sim}{v}$, giving the system

$$\underset{\sim}{u}_t = \underset{\sim}{F}(\underset{\sim}{u}) + K\,\underset{\sim}{u}_{xx}$$

$$\underset{\sim}{v}_t = \nabla \underset{\sim}{F}(\underset{\sim}{u})\underset{\sim}{v} + K\,\underset{\sim}{v}_{xx}. \tag{2.14}$$

Introduce the functions

$$G_i = \frac{1}{2}u_i^2 + v_i - k$$

$$\hat{G}_i = \frac{1}{2}u_i^2 - v_i - k, \quad i = 1, \ldots, N. \tag{2.15}$$

It will be shown that if k is chosen sufficiently large, then G_i, $\hat{G}_i < 0$ for all i when $t \geq 0$, so that $-k + \frac{1}{2}u_i^2 < u_{ix} < k - \frac{1}{2}u_i^2$. (Notice that $d_i > 0$ for all i is essential in the proof, another example of an argument which does not carry over to a singular diffusion matrix.)

Assume k is sufficiently large that G_i, $\hat{G}_i < 0$ for all i at $t = 0$. If G_i, $\hat{G}_i < 0$ for all t, we are finished, so let t_o be the time at which some component first equals 0. First assume some $G_i = 0$. Then the precise meaning of t_o is

for $t < t_o$, we have G_i, $\hat{G}_i < 0$ for all i, all x;

for $t = t_o$, we have G_i, $\hat{G}_i \leq 0$ for all i, all x,

and some $G_j = 0$ at $x = x_o$. (2.16)

At (x_o, t_o), G_j is nondecreasing in the t-direction and has a local maximum in the x-direction, so

$$G_j = \frac{1}{2} u_j^2 + v_j - k = 0; \tag{2.17a}$$

$$(G_j)_t = u_j(d_j\, u_{jxx} + F_j(\underset{\sim}{u})) + (d_j\, v_{jxx} +$$

$$(\nabla \underset{\sim}{F}(\underset{\sim}{u})v)_j) \geq 0; \tag{2.17b}$$

$$(G_j)_{xx} = u_{jx}^2 + u_j u_{jxx} + v_{jxx} \leq 0. \tag{2.17c}$$

Substitution of (2.17c) and (2.17a) into the expression for $(G_j)_t$ gives

$$(G_j)_t \leq -d_j(k - \frac{1}{2} u_j^2)^2 + u_j\, F_j(\underset{\sim}{u})$$

$$+ \sum_{i=1}^{N} \frac{\partial F_j}{\partial u_i} (\underset{\sim}{u})\, v_i. \tag{2.18}$$

Now, all u_i's are bounded by (2.13c) and v_i's are linearly bounded in k by (2.16), so if we had initially chosen k sufficiently large that the quadratic term $-d_j k^2$ dominated in (2.18), then $(G_j)_t < 0$ would result, contradicting $(G_j)_t \geq 0$ in (2.17b).

Therefore, the assumption some $G_i = 0$ at t_o is false. The same argument, however, goes through to show $\hat{G}_i = 0$ at t_o is also impossible, so $\underset{\sim}{v}$ stays bounded.

The boundary conditions in Chueh, Conley, and Smoller are basically that the values $\underset{\sim}{u}(\underset{\sim}{x},t)$, $\underset{\sim}{x}$ on the boundary of the spatial domain, be bounded within the interior of the invariant set for $\underset{\sim}{u}$. Conway and Smoller (1977) have extended the boundedness results to include Neumann boundary conditions. Conway, Hoff, and Smoller (1978) showed that, for reaction-diffusion systems possessing positively-invariant sets (so solutions remain bounded) and with Neumann boundary conditions on sufficiently small domains (so diffusion is strongly felt over the domain), solutions decay to spatially homogeneous functions (necessarily solutions of the kinetic system, such as constants or limit cycles). The paper illustrates how a general boundedness result can lead to estimates of decay rates and eventually to stability results for particular solutions. Incidentally, their proof is to use the boundedness of solutions plus Neuman boundary conditions to show that—on sufficiently small spatial domains D—

$$\int_D ||\nabla_x \underset{\sim}{u}||^2 \, dx \leq c_1 \exp(-c_2 t). \tag{2.19}$$

By rather intricate arguments and certain results from the literature, this L_2-bound is converted to a similar result for L_∞:

$$\sup_D ||\nabla_x \underset{\sim}{u}|| \leq c_3 \exp(-c_4 t),$$

which definitely forces $\underset{\sim}{u}$ to converge to a spatially homogeneous solution. Their derivation of (2.19) easily carries over to the system with periodic boundary conditions (2.13), and (2.19) together with the boundedness of $||\underset{\sim}{u}_x||$ immediately gives $||\underset{\sim}{u}_x|| \to 0$ as $t \to +\infty$, forcing a spatially homogeneous solution.

A simple form of this type of geometric boundedness argument was also used by Evans and Shenk (1970). For systems of the form

$$V_t - V_{xx} = f(V, \underset{\sim}{W})$$

$$\underset{\sim}{W}_t = \underset{\sim}{g}(V, \underset{\sim}{W})$$

where V is a scalar function and $\underset{\sim}{W}$ is a vector function, they showed that, for $E_1 < E_2$, $f(E_1, \underset{\sim}{W}) > 0$ and $f(E_2, \underset{\sim}{W}) < 0$ and $E_1 < V(x,0) < E_2$ implies $E_1 < V(x,t) < E_2$ for $t \geq 0$.

Problems Considered in this Thesis

In discussing reaction-diffusion systems in the first two sections, I have occasionally pointed out certain questions, arising either explicitly in the literature or as natural questions to ask, which are studied in this thesis. This section will discuss the contents of this thesis directly.

The literature of reaction-diffusion systems contains much work on stationary states (both spatially homogeneous and inhomogeneous) and traveling waves (periodic waves, traveling fronts, solitary waves). This thesis is basically concerned with the limit cycle of the kinetic system as a spatially homogeneous, time-periodic solution of the reaction-diffusion system (1.1); relatively little work has appeared in the literature on this topic. Other results arising in the course of the limit cycle study are also given.

The next section of this first chapter studies classes of reaction-diffusion systems for which explicit transient solutions occur, solutions representing transitions between stationary states and periodic traveling waves. Some of the general results of the second section will be used to derive properties of these classes of equations, which have appeared in Cope (1979).

The second chapter studies the linear stability of the limit cycle as a solution of the reaction-diffusion system. The study is motivated by Turing's result that a kinetically stable stationary state can become unstable when diffusion is added; we ask: can a kinetically stable limit cycle become unstable when diffusion is added? (The question has also been brought up by Othmer (1977) and Kopell and Howard (1973)). The variational equation about the limit cycle reduces to a Floquet system with wave number k^2 appearing as a parameter. Perturbations based on the Floquet representation of the solutions give solutions for small k^2 and large k^2. The limit cycle can become unstable to small k^2, and explicit examples of such systems are constructed and examined numerically (using Lees' method, discussed in chapter V). If the diffusion matrix is singular, the limit cycle can become unstable to large k^2 also (when the diffusion matrix is nonsingular, it is well-known that the limit cycle is stable to all large k^2). These results have appeared in Cope (1980).

A point near a stable limit cycle $\underset{\sim}{U}(t)$ ($\underset{\sim}{U}(0)$ specified) gives a trajectory $\sim \underset{\sim}{U}(t + \phi)$ as $t \to +\infty$; ϕ is the <u>asymptotic phase</u> of the point. Winfree has named a surface of points with the same asymptotic phase an <u>isochron</u>. Constructive existence proofs have been given for isochrons, but they are based on contractive mappings, specifically the iterative solution of nonlinear integral equations on $[0,\infty)$, and are quite awkward for actual computation. Winfree (1978) has suggested computation of isochrons as a research problem. This problem is studied in chapter III. The computation is by a series expansion based on Liapunov's construction of trajectories near a stable critical point—the linearized system has exponentially-decaying solutions and the actual solution is a power series in these exponentials. The linearized system near the limit cycle has 1 periodic solution and the rest exponentially-decaying, and trajectories near the limit cycle can be expressed as a power series in these exponentials. The coefficients of the series are T-periodic functions and each has to be calculated by a quadrature of preceeding coefficients. A particularly accurate and efficient means of carrying out such integrations, based on extrapolation formulas and the periodicity of all functions concerned, is given. Numerical calculations are shown to illustrate results. Convergence of the expansion is proven.

The fourth chapter considers the calculation of asymptotic phase for a reaction-diffusion system. Here initial data is taken to have the form $\underset{\sim}{U}(0) + \underset{\sim}{f}(\underset{\sim}{x})$, where $\underset{\sim}{f}(\underset{\sim}{x})$ is a small periodic perturbation, and if the limit cycle is stable as a solution of the diffusion system, this initial data should evolve to $\underset{\sim}{U}(t + \phi)$, ϕ constant, as $t \to +\infty$. The problem considered is to find ϕ, given the initial perturbation $\underset{\sim}{f}(\underset{\sim}{x})$. A formal multi-scaling expansion is derived for the case of long spatial scales (i.e., perturbations corresponding to small wave number). (This expansion, or at least its first term, has also been used in Howard and Kopell (1977) and in Neu (1979) with regard to other behavior in reaction-diffusion systems.) It is shown that the expansion leads to exactly the same characterization of instability to small wave numbers k^2 as obtained in the linear stability study in chapter II, that the expansion is well-defined to all orders, and that a simple expression for the first-order term of ϕ in terms of $f(x)$ can be obtained.

The fifth chapter compares the predicted results of the formal multi-scaling expansion of chapter IV with numerical results for two specific equations, a $\lambda - \omega$ system and a system occurring in Cohen, Hoppenstaedt, and Miura (1977). The numerical work is based on Lees' method, an especially efficient finite difference scheme for parabolic equations. The method itself is described and particular problems arising in these calculations are discussed. These problems are that one must start with a small perturbation ($O(\epsilon)$) of the limit cycle, integrate until this initial perturbation dies away to a constant phase shift (and the decay rate is like $\exp(O(\epsilon)t)$), and then measure that phase shift, which is itself $O(\epsilon)$. These problems can, however, be overcome and the numerically found phase shifts are in good agreement with the predicted ones.

Chapter V is actually in two parts. The first part is simply the numerical check of the results of chapter IV, as just described. The second part is concerned with a question of numerical analysis: the nonlinear stability of finite difference schemes for parabolic systems. Finite difference schemes are generally rated as (numerically) stable or unstable according to their behavior when applied to linear systems with constant coefficients, because the resulting difference equations can be solved exactly and analyzed. Very little is known about numerical stability of finite difference schemes applied to nonlinear PDEs. I became interested in this question (after it arose in a numerical analysis seminar given by J. Varah) because the boundedness arguments of Chueh, Conley, and Smoller (1977) seemed to carry over directly to the finite difference equations. They did, but the resulting restrictions for nonlinear numerical stability were generally of the form $\Delta t = O(\Delta x^2)$, even for Lees' method, which seemed overly restrictive considering how well Lees' method worked in practice. Further work, concentrating on direct estimates, eventually led to a nonlinear numerical stability restriction of $\Delta t = O(\Delta x)$ on Lees' method.

Finally, in the sixth chapter, the construction of periodic traveling waves as perturbations off the limit cycle is studied. A series expansion, based on a direct substitution into the equations for the traveling wave, has been given by Wasow (1976); he only claimed the expansion asymptotic to the true solution. Kopell and Howard (1973) used a rather curious change of variable on the equations for the traveling wave, then rewrote the equations as an integral equation and proved the integral equation possessed a periodic solution by a contractive mapping. The basic question of chapter VI is: why should a series expansion, such as Wasow's, be only asymptotic when the integral equation formulation can be shown convergent? The answer is that a convergent series expansion can be found, but the proof involves regrouping the terms of the series in an unexpected fashion and using an interesting property, due to Kopell and Howard, of the solutions of Floquet systems. In other words, chapter VI gives an alternate proof of the existence of periodic traveling waves, using a series expansion instead of the integral equation of Kopell and Howard.

In short, this thesis is basically a study of the limit cycle as a solution of (1.1) (Chapters II, IV, first half of V, VI), together with related results which arose in the course of the study (last half of chapters I and V, chapter III). Appendix I gives Lemmas A,B,C, and D, which are used throughout the thesis. Appendix II is a convergence proof for the expansion developed in Chapter III. Appendices III and IV contain further work on the expansion developed in Chapter IV.

Reaction-Diffusion Equations with Explicit Traveling Wave and Transient Solutions

The $\lambda-\omega$ systems (2.7) with explicit traveling wave solutions have been quite important in the study of reaction-diffusion equations. Considerable insight results from examining ideas within this simple class of equations with its explicit traveling waves. For example, Kopell and Howard (1973) solved exactly the linear stability problem for the traveling waves of the $\lambda-\omega$ systems, thereby giving evidence for the stability of large amplitude traveling waves (see last section). Greenberg's proof (1978) of the existence of circular wave solutions is for $\lambda-\omega$ systems, not reaction-diffusion systems in general. Similarly, Cohen, Neu, and Rosales (1978) proved the existence of spiral wave solutions only for $\lambda-\omega$ systems. (The extension of these results to more general systems is still an open problem, although Greenberg (1976) gave a carefully done formal expansion for circular waves for reaction-diffusion equations in general.)

This section shows various types of behavior of solutions in reaction-diffusion equations by giving explicit solutions to two classes of equations.

The first class of equations differs from λ-ω systems in permitting nonscalar diffusion matrices and kinetic terms which are not of λ-ω form. These systems possess an explicit periodic traveling wave solution of the form $(u,v) = (R_0 \cos\psi,\ R_0 \sin\psi)$, $\psi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x}$ where $\underset{\sim}{k}$ is a constant vector. A new type of solution, transition from (or to) a stationary state to (or from) the periodic traveling wave, also occurs; its form is $(u,v) = (R(\psi) \cos\psi,\ R(\psi) \sin\psi)$, $\psi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x}$, with $0 \leq R(\psi) \leq R_0$.

To illustrate the use of material in the previous section, a subclass of these equations will be studied in detail. It will be shown (using the Poincaré-Bendixson Theorem) that these systems possess a stable limit cycle for the kinetic equations. From the results of Kopell and Howard (1973), discussed in the last section, it follows that a family of periodic traveling waves exists for the full reaction-diffusion equations. The same properties used to show the existence of the limit cycle solution enable the results of Chueh, Conley, and Smoller (1977), discussed in the second section, to be applied so that appropriately bounded initial data produce solutions remaining bounded for all time.

The second class of equations is a special set of λ-ω systems. This class also possesses solutions representing a transition between a stationary state and a periodic traveling wave, but these transients have the form $(u,v) = (R(\psi_1) \cos\psi_2,\ R(\psi_1) \sin\psi_2)$, $\psi_i = b_i t - \underset{\sim}{k}_i\cdot\underset{\sim}{x}$, $i = 1,2$ where $\underset{\sim}{k}_1$ and $\underset{\sim}{k}_2$ are constant vectors. The amplitude $R(\psi_1)$ and phase ψ_2 propagate in different directions!

It is interesting to connect these transient solutions with the linear stability analysis of periodic traveling waves for $\lambda-\omega$ systems discussed in the second section. (This second class of equations satisfies the mild assumptions made in that analysis.) Kopell and Howard derived an exact condition (2.10) for the linear stability of traveling waves in $\lambda-\omega$ systems. The transient solutions, as developed here, represent transitions between the unstable stationary state (0,0) and periodic traveling waves of various amplitudes. I would have expected in the case of a stable traveling wave that transitions were always from (0,0) to the wave, while the transition could go either way betwenn (0,0) and unstable traveling waves. Surprisingly, this is not the case. The second class of equations contains solutions representing a transition <u>from</u> linearly stable traveling waves <u>to</u> the linearly unstable solution (0,0).

Finally, analogies can be drawn between these explicit solutions and circular and spiral wave solutions. If one considers circular waves propagating out from a point, then at large distances from the point the circular waveis asymptotic to a plane wave propagating inthe radial direction. At the edge of the circular wave, the behavior in the direction of propagation may be a transition from a stationary state to periodic behavior, corresponding to the transients of the first class of equations. The transients of the second class of equations with their amplitude and phase propagating in different directions suggests the behavior at the edge of a spiral wave: the phase may be propagating along a radial line with a transition from a stationary state to periodic behavior, but the "spiralness" is due to the amplitude propagating in a slightly off-radial direction.

The first class of equations can be generated as follows. The substitution $(u,v) = (R\cos\psi,\ R\sin\psi)$ into (2.1) yields

$$\begin{bmatrix} R_t \\ \psi_t \end{bmatrix} = \begin{bmatrix} R\,\lambda(R,\psi) \\ \omega(R,\psi) \end{bmatrix} + \begin{bmatrix} 1+\alpha\cos 2\psi & -\alpha R\sin 2\psi \\ -\frac{\alpha}{R}\sin 2\psi & 1-\alpha\cos 2\psi \end{bmatrix}$$

$$\begin{bmatrix} \nabla^2 R - R\,|\nabla\psi|^2 \\ \frac{2}{R}\nabla R\cdot\nabla\psi + \nabla^2\psi \end{bmatrix}, \quad |\alpha| \le 1, \tag{4.1a}$$

where λ,ω are related to F,G by

$$\begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} = \begin{bmatrix} u & -v \\ v & u \end{bmatrix}\begin{bmatrix} \lambda \\ \omega \end{bmatrix}, \quad \begin{bmatrix} \lambda(R,\psi) \\ \omega(R,\psi) \end{bmatrix} = \frac{1}{R^2}\begin{bmatrix} u & v \\ -v & u \end{bmatrix}\begin{bmatrix} F \\ G \end{bmatrix}. \tag{4.1b}$$

Assume solutions of the form $\psi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x}$, $R = R(\psi)$ so that (4.1) gives two ODE's for R. Without loss of generality, $k^2 = 1$ can be assumed. The two ODE's are $(R' = {}^{dR}/_{d\psi})$:

$$\begin{bmatrix} b\,R' \\ b \end{bmatrix} = \begin{bmatrix} R\lambda \\ \omega \end{bmatrix} + \begin{bmatrix} 1+\alpha\cos 2\psi & -\alpha R\sin 2\psi \\ -\frac{\alpha}{R}\sin 2\psi & 1-\alpha\cos 2\psi \end{bmatrix}\begin{bmatrix} R'' - R \\ 2\frac{R'}{R} \end{bmatrix}. \tag{4.2}$$

The function $R(\psi)$ must satisfy two second-order ODE's simultaneously so it will necessarily satisfy a first order ODE, which will be written as

$$R' = -R\ P(R,\psi). \tag{4.3}$$

The idea is to define λ, ω in terms of P so that the two equations of (4.2) do in fact have a common solution. Substitution of (4.3) into (4.2) gives this consistency condition on λ, ω as

$$\begin{bmatrix} \lambda \\ \omega \end{bmatrix} = \begin{bmatrix} -bP \\ b \end{bmatrix} + \begin{bmatrix} 1 + \alpha \cos 2\psi & -\alpha R \sin 2\psi \\ -\frac{\alpha}{R} \sin 2\psi & 1 - \alpha \cos 2\psi \end{bmatrix}$$

$$\begin{bmatrix} 1 + P_\psi - RP_R P - P^2 \\ 2P \end{bmatrix}. \tag{4.4}$$

The results are summed up as

LEMMA 1. Let $R(\psi)$ be any solution of (4.3). Then the system

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} -bP + (1 + \alpha)Q & -b - 2(1 + \alpha) \\ b + 2(1 - \alpha)P & -bP + (1 - \alpha)Q \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} (1 + \alpha)\nabla^2 u \\ (1 - \alpha)\nabla^2 v \end{bmatrix} \tag{4.5a}$$

with $Q = 1 + P_\psi - RP_R P - P^2$, has the solution

$$(u,v) = (R(\psi)\cos\psi,\ R(\psi)\sin\psi) \text{ with } \psi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x},\ k^2 = 1. \quad (4.5b)$$

The systems (4.5a) are generated by choosing the arbitrary function P. They differ from λ-ω systems in the nonscalar diffusion matrix and in permitting more general kinetic terms. For instance, if $P = P(R)$, then Q depends only on R and the kinetic terms will have λ-ω form; if P is any polynomial in u,v, then Q is also a polynomial (because $P_\psi = -vP_u + uP_v$ and $RP_R = uP_u + vP_v$) and systems not of λ-ω form can occur.

If $P = P(R)$ and $\alpha = 0$, then (4.5a) becomes a λ-ω system and it is instructive to compare the results of Lemma 1 with the usual solutions. Choosing $P(R,\psi) = a - R$, $a > 0$, $\alpha = 0$ and $b = -3a$ reduces (4.5a) to the following special case

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} 1 + 2(a^2 - R^2) & a + 2R \\ -a - 2R & 1 + 2(a^2 - R^2) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} \nabla^2 u \\ \nabla^2 v \end{bmatrix}. \quad (4.6)$$

From (2.8), the usual λ-ω solutions are

$$\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} R_o \cos(-(a + 2R_o)t - \underset{\sim}{k}\cdot\underset{\sim}{x}) \\ R_o \sin(-(a + 2R_o)t - \underset{\sim}{k}\cdot\underset{\sim}{x}) \end{bmatrix} \text{ with } k^2 = 1 + 2(a^2 - R_o^2). \quad (4.7)$$

From Lemma 1, we have the solutions (from $R' = -R(a - R)$)

$$(u,v) = (R(\psi)\cos\psi,\ R(\psi)\sin\psi); \tag{4.8a}$$

$$\psi = -3a - \underset{\sim}{k}\cdot\underset{\sim}{x},\quad k^2 = 1; \tag{4.8b}$$

$$R(\psi) = \begin{cases} a & \text{or} \\ \dfrac{a}{1 + \exp\,(a(\psi+\psi_0))}, & \psi_0 = \text{arbitrary constant.} \end{cases} \tag{4.8c}$$

Of these latter solutions, one is a standard traveling wave of λ-ω type (amplitude $R_0 = a$ in (4.7)), and the others are transient solutions representing a transition from the 0-solution to the traveling wave $R_0 = a$ (since $\exp(-3a^2t)$ occurs in (4.8c)). Incidentally, if the stability criterion (2.10) is applied to the wave $R_0 = a$, then the wave is linearly stable if

$$1 + \frac{1}{4a^2} - a^2 \leq 0.$$

The transition from 0 to the traveling wave is therefore a transition from one linearly unstable solution to another for small a, and from a linearly unstable solution to a linearly stable one for large a.

The kinetic equations for a λ-ω system have a rather simple phase plane: the origin is the only critical point (except for the degenerate case of a circle of critical points) and the occurrence of limit cycles is trivial to check. The kinetic equations for systems

(4.5a) are not quite so transparent, and it will now be shown that they do show interesting behavior, such as limit cycles.

Notice that if the kinetic equations have the origin as an unstable critical point, if the origin is the only critical point, and if all solutions are bounded as $t \to +\infty$, then the Poincaré-Bendixson Theorem (Coddington and Levinson, 1955) gives a stable limit cycle. These three conditions will be used to prove the following lemma giving sufficient conditions on P for the kinetic equations of (4.5a) to possess limit cycles.

LEMMA 2. Let $P(u,v)$ be polynomial in u,v, and $b \neq 0$, $|\alpha| \neq 1$ in the kinetic equations of (4.5a).

(a) If $P(0,0)$ is sufficiently close to 0, then the origin is an unstable critical point (in particular, an unstable spiral if $\alpha^2 > b^2$).

(b) If $|\alpha b| < 1 - \alpha^2$ and either

(1) $b > 0$ and $P(u,v) > - b(1 - \alpha)/2(1 - \alpha^2 + |\alpha b|)$ or

(2) $b < 0$ and $P(u,v) < - b(1 - \alpha)/2(1 - \alpha^2 + |\alpha b|)$,

then the origin is the unique critical point.

(c) If $P(u,v)$ is nonzero for all sufficiently large R, then all solutions of the kinetic equations of (4.5a) are bounded as $t \to +\infty$.

(d) If the hypotheses of (a), (b), (c) hold, then the kinetic equations of (4.5a) possess at least one stable limit cycle.

PROOF. (a) Since P is polynomial in u,v and $P_\psi = -vP_u + uP_v$, $RP_R = uP_u + vP_v$, then $Q(0,0) = 1 - P^2(0,0)$, where $Q(u,v)$ is defined from

$P(u,v)$ by Lemma 1. If $P(0,0) = 0$, then the linearized kinetic equations (4.5a) about the origin have the coefficient matrix

$$\begin{bmatrix} 1+\alpha & -b \\ b & 1-\alpha \end{bmatrix}$$

with eigenvalues $1 \pm (\alpha^2 - b^2)$. Since $b^2 > 0$ by hypothesis and $\alpha^2 < 1$, these eigenvalues are either strictly positive (if $\alpha^2 > b^2$) or complex with positive real part ($\alpha^2 < b^2$). By continuity the instability persists if $P(0,0)$ is close to 0. (b) Assume $(u_o,v_o) \neq (0,0)$ is a critical point for the kinetic equations of (4.5a). Eliminating $Q(u_0,v_0)$ from the two rest state equations $u' = 0$, $v' = 0$ gives the necessary condition on $P_0 = P(u_0,v_0)$:

$$\begin{aligned} 2\,[(1-\alpha^2)(u_o^2 + v_o^2) - 2\,\alpha\, b\, u_o\, v_o]\, P_o \\ = -b[(1+\alpha)\ u_o^2 + (1-\alpha)\ v_0^2] \,. \end{aligned}$$

Setting $(u_o,v_o) = (R_o \cos\theta_o\,,\ R_o \sin\theta_o)$, the resulting equation is

$$2[1 - \alpha^2 - \alpha\, b \sin 2\theta_o]\ \ P_o = -b[1 + \alpha \cos 2\theta_o],$$

and the assumption $|\alpha b| < 1 - \alpha^2$ insures the coefficient of P_0 is positive. Since

$$0 < \frac{1 - \alpha}{1 - \alpha^2 + |\alpha b|} \leq \frac{1 + \alpha \cos 2\theta_o}{1 - \alpha^2 - \alpha b \sin 2\theta_o} \leq \frac{1 + \alpha}{1 - \alpha^2 - |\alpha b|}$$

then at this critical point (u_0, v_0)

$$\frac{-b(1 - \alpha)}{2(1 - \alpha^2 + |\alpha b|)} \geq P_o \geq \frac{-b(1 + \alpha)}{2(1 - \alpha^2 - |\alpha b|} \quad \text{if} \quad b > 0,$$

and if $b < 0$ the inequalities reverse. But these inequalities contradict the assumption on $P(u,v)$. (c) $P(u,v)$ is nonzero for all sufficiently large R iff the homogeneous polynomial consisting of the highest degree terms of P is positive-definite (or negative-definite). This definiteness can occur only if the polynomial has even degree, so $P(u,v) = H_{2n}(u,v) + A(u,v)$, where $A(u,v)$ has degree $< 2n$ and $H_{2n}(u,v)$ is a positive- (negative-) definite homogeneous polynomial of degree $2n$. Noting $RH_{2n,R} = 2n\, H_{2n}$ and letting $R \to +\infty$ in the kinetic equations of (4.5a) gives

$$\begin{bmatrix} F \\ G \end{bmatrix} \sim -(2n + 1)\ H_{2n}^2 \begin{bmatrix} (1 + \alpha)u \\ (1 - \alpha)v \end{bmatrix}. \tag{4.9}$$

Since $|\alpha| \neq 1$, this vector field always points inwards for sufficiently large R and all kinetic solutions must be bounded as $t \to +\infty$.

(d) It is only necessary to note that (a), (b), (c) are all compatible conditions, in particular $P(0,0)$ close to 0 is compatible with the bound on P in (b). Q.E.D.

The proof of boundedness for solutions to the kinetic system (Lemma 2c) immediately gives a proof of boundedness of solutions of the reaction-diffusion system using the results of Chueh, Conley, and Smoller discussed in the last section.

LEMMA 3. In (4.5a), let $P(u,v)$ be polynomial in u and v, $|\alpha| \neq 1$. and $P(u,v)$ be nonzero for all sufficiently large R. Then, for any smooth initial data $u(\underset{\sim}{x},o)$, $v(\underset{\sim}{x},o)$ of (4.5a), there exists a constant B such that $|u(\underset{\sim}{x},t)|$, $|v(\underset{\sim}{x},t)| \leq B$ for $t \geq 0$.

PROOF. Under these assumptions, equation (4.9) holds. Hence any box with sides parallel to the (u,v)-axes is an invariant set if it is sufficiently large, since (4.9) shows the kinetic vector field must point inwards on the perimeter of any sufficiently large box. Given initial data $u(\underset{\sim}{x},o)$, $v(\underset{\sim}{x},o)$, in the (u,v)-plane pick a $2B \times 2B$ square centered at the origin with sides parallel to the axes such that $|u(\underset{\sim}{x},o)|$, $|v(\underset{\sim}{x},o)| \leq B$, then the square forms an invariant set. By Theorem 1 the solution satisfies the same bound for all time. Q.E.D.

As an example of (4.5a) with the equations not of $\lambda-\omega$ form, consider $P(u,v) = c - H_{2n}(u,v)$, where c is a positive constant and $H_{2n}(u,v)$ is a positive-definite, homogeneous polynomial in u,v of degree 2n. This choice for P leads to systems which are not of $\lambda-\omega$ form unless H_{2n} reduces to a function of R alone.

If c is sufficiently small and α, b are appropriately related in (4.5a), then Lemma 2 applies and the kinetic equations of (4.5a) possess a stable limit cycle.

By the results of Kopell and Howard (1973), discussed in the last section, a family of periodic traveling waves exists.

By Lemma 3, this choice of P implies that initially bounded solutions of (4.5a) are bounded for all time.

Equation (4.5b) for the amplitude $R(\psi)$ of the traveling wave becomes a Bernoulli equation with solution

$$R^{-2n} = \exp(2nc\psi)\left[\hat{c} - 2n\int_0^{\psi} \exp(-2ncs)\, H_{2n}(\cos s, \sin s)ds\right],$$

$$\hat{c} \text{ arbitrary constant.} \tag{4.10}$$

The behavior of this solution can be found using Lemma A in Appendix 1; the lemma gives the results of integrating an exponential against a periodic function. By Lemma A.2, we have

$$\int_0^{\psi} \exp(-2ncs)\, H_{2n}(\cos s, \sin s)ds = \exp(-2nc\psi)h(\psi) - h(0),$$

where $h(\psi)$ is a 2π-periodic function and, by Lemma A.4 and $H_{2n}(\cos s, \sin s) > 0$, it follows that $h(\psi) < 0$. Consequently,

$$R^{-2n} = \exp(+2nc\psi)\,[\hat{c} + 2n\, h(0)] - 2n\, h(\psi). \tag{4.11}$$

The exponential part of the expression is always positive, and so is $-2n\ h(\psi)$. Therefore $R(\psi)$ is finite for all ψ and varies from a purely periodic function as $\psi \to -\infty$ to 0 as $\psi \to +\infty$. The limiting periodic wave is given by choosing $\hat{c}$ so that the coefficient of the exponential term is 0.

The corresponding solutions $(u,v) = (R(\psi)\cos\psi,\ R(\psi)\sin\psi)$ with $\psi = bt - \underset{\sim}{k}\cdot\underset{\sim}{x}$, $k^2 = 1$ represent transient solutions changing from 0 to a purely periodic wave (for $b < 0$; for $b > 0$ the transition is from the periodic wave to 0). In contrast to $\lambda-\omega$ systems, the amplitude $R(\psi)$ of this periodic wave is not constant. There is a 1-parameter family of transients; the parameter $\hat{c}$ represents a phase shift between the periodic solution and the exponential part.

The second class of equations will now be constructed and studied.

In the preceding examples, only a single periodic wave is found explicitly, together with a corresponding family of transient solutions. It is natural to look for examples where transient solutions can be calculated for a family of periodic waves. The trick in getting such solutions is to let the amplitude and phase portions of the solution correspond to traveling waves propagating in different directions with different velocities. (In this sense, the solutions u,v correspond to a nonlinear superposition of traveling waves.)

The second class of equations of $\lambda-\omega$ systems (2.7a,b) with:

$$\begin{aligned}
&\text{(a)} \quad \lambda(R) = -(R^n - a)(R^n - b), \quad n > 0; \\
&\text{(b)} \quad \omega(R) = d(R^n - c); \\
&\text{(c)} \quad |a| < b \text{ and } b \text{ positive}; \\
&\text{(d)} \quad \frac{d^2(n+1)}{4} < \frac{(b-a)^2}{4} = \max \lambda(R).
\end{aligned} \tag{4.12}$$

The usual traveling wave solutions are given by (2.8). We look for solutions of the form $(u,v) = (R(\theta)\cos\psi,\ R(\theta)\sin\psi)$, with $\psi = b_o t - \underset{\sim}{k}_o \cdot \underset{\sim}{x}$, $b_o = \omega(R_o)$, $k_o^2 = \lambda(R_o)$ -- as in the usual solution with amplitude R_o -- and set $\theta = b_1 t - \underset{\sim}{k}_1 \cdot \underset{\sim}{x}$, to be determined:

$$\begin{aligned}
&\text{(a)} \quad 0 = R(\lambda(R) - \lambda(R_o)) - b_1 R' + k_1^2 R'' \\
&\text{(b)} \quad 0 = \omega(R) - \omega(R_o) + \frac{2}{R} \underset{\sim}{k}_o \cdot \underset{\sim}{k}_1 R'
\end{aligned} \tag{4.13}$$

If $\underset{\sim}{k}_o \cdot \underset{\sim}{k}_1 = 0$, the equations reduce to the usual traveling waves (2.8). Assume $\underset{\sim}{k}_o \cdot \underset{\sim}{k}_1 \neq 0$; without loss of generality, $k_1^2 = 1$ can be assumed since this simply fixes a space scale for (4.13). At this point we have chosen b_o, but not b_1, and the lengths of $\underset{\sim}{k}_o$ and $\underset{\sim}{k}_1$, but not their directions. Repeated substitution of (4.13b) into (4.13a) until all derivatives $dR/d\theta$ are eliminated and the use of (4.12) eventually yields as a consistency condition the following polynomial equation for R:

$$\left[(n+1)d^2 - (2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1)^2\right]R^{2n} + \left[(2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1)^2(a+b) + 2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1\, db_1 - (n+2)d^2R_o{}^n\right]R^n + \left[((2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1)^2 + d^2)R_o^n - (2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1)^2(a+b) - 2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1\, db_1\right]R_o^n = 0.$$

Setting the coefficients of R^{2n}, R^n, and R^o to zero gives conditions determining $\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1$ and b_1. Specifically,

$$(2\,\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1)^2 = (n+1)\,d^2, \tag{4.14a}$$

and by condition (4.12d)

$$\left(\frac{\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1}{|\underset{\sim}{k}_o||\underset{\sim}{k}_1|}\right)^2 = \frac{(n+1)d^2}{4\,\lambda(R_o)} \le 1,$$

so the cosine of the angle between $\underset{\sim}{k}_o$ and $\underset{\sim}{k}_1$ is well-defined. Next,

$$b_1 = -\frac{2\underset{\sim}{k}_o\cdot\underset{\sim}{k}_1}{d}\left[a + b - \frac{n+2}{n+1}R_o^n\right]. \tag{4.14b}$$

These conditions automatically make the coefficient of R^o equal to zero, so the third condition is redundant. Summarizing these results as a lemma:

LEMMA 4. For the λ-ω system with $\lambda(R)$, $\omega(R)$ given by (4-12), assume:

(a) $R_o > 0$ is an arbitrary constant;

(b) $\psi = b_o t - \underset{\sim}{k}_o \cdot \underset{\sim}{x}$ with $b_o = \omega(R_o)$, $\underset{\sim}{k}_o$ an arbitrary vector with $k_o^2 = \lambda(R_o)$;

(c) $\theta = b_1 t - \underset{\sim}{k}_1 \cdot \underset{\sim}{x}$ with $\underset{\sim}{k}_1$ a unit vector satisfying (4.14a) and b_1 satisfying (4.14b);

(d) $R(\theta)$ satisfies

$$\frac{dR}{d\theta} = \frac{-d}{2\underset{\sim}{k}_o \cdot \underset{\sim}{k}_1} R\,(R^n - R_o^n)\ .$$

Then $(u,v) = (R(\theta)\cos\psi,\ R(\theta)\sin\psi)$ is a solution of the λ-ω system defined by (4.12).

The equation in Lemma 4d is an easily solvable Bernoulli equation, and it is clear from its form alone that (bounded) solutions of $R(\theta)$ represent a transition between amplitudes 0 and R_o. If the position $\underset{\sim}{x}$ is assumed fixed, so $d\theta = b_1\,dt$ in Lemma 4c, and (4.12b) is combined with Lemma 4d, we have

$$dR = R\,(R^n - R_o^n)\,(a + b - \frac{n+2}{n+1} R_o^n)\,dt.$$

Since $0 < R(\theta) < R_o$, the direction of the transition depends on R_o (note $a + b > 0$ by (4.12c)):

Set $\rho = [(n+1)(a+b)/(n+2)]^{1/n}$.

If $R_o > \rho$, then the solution given in Lemma 4 is a transition from 0 to a solution with amplitude R_o; if $R_o < \rho$, then the transition is from amplitude R_o to 0. Roughly, for large R_o the transition in amplitude is from 0 to R_o, and for small R_o the transition is from R_o to 0 — a conclusion consistent with Kopell and Howard's results of linearly stable large amplitude waves and unstable small amplitude waves.

However, the value of R_o separating the two types of transition does not quite match up with Kopell and Howard's result. Defining (by (4.12))

$$\begin{aligned} F(R) &= 4\lambda(R)\left[1 + \left(\frac{\omega'(R)}{\lambda'(R)}\right)^2\right] + R\lambda'(R) \\ &= -4(R^n - a)(R^n - b)\left[1 + \left(\frac{d}{2R^n - a - b}\right)^2\right] \\ &\quad - nR^n\,(2R^n - a - b), \end{aligned} \tag{4.16}$$

Kopell and Howard found that the $\lambda-\omega$ traveling wave with amplitude $R_o > 0$ is linearly stable iff $F(R_o) \leq 0$. Examining $R_o = \rho$, we find

$$F(\rho) = -4\left(b - \frac{a+b}{n+2}\right)\left(a - \frac{a+b}{n+2}\right)\left[1 + \left(\frac{d}{a+b} \quad \frac{n}{n+2}\right)^2\right]$$

$$- \frac{n^2(n+1)}{(n+2)^2}(a+b)^2 .$$

As $n \to +\infty$, then $\rho \to 1$ and $F(\rho) \sim -n(a+b)^2 < 0$. Consequently, there is an $\epsilon > 0$, independent of n, such that

(a) for R_o in the interval $1 - \epsilon < R_o < 1 + \epsilon$, $F(R_o) < 0$ and the traveling waves of amplitude R_o are linearly stable by Kopell and Howard's criterion, and

(b) the interval $1 - \epsilon < R_o < 1 + \epsilon$ contains values of $R_o < \rho$ and $R_o > \rho$, so the transitions given by the explicit solutions of Lemma 4 are <u>from</u> the linearly stable waves of amplitude R_o <u>to</u> the linearly unstable 0-solution.

Strange as it may be, of course, the behavior does not contradict the linear stability of the traveling wave since that stability is derived on the basis of a small perturbation of the solution, while the transient is a small perturbation in one region of space but O(1) in another.

CHAPTER II

STABILITY OF LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS

Introduction

Consider the general reaction-diffusion system in two dependent variables, written in normalized form as

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} + \begin{bmatrix} 1+\alpha & \delta_2 \\ \delta_1 & 1-\alpha \end{bmatrix} \begin{bmatrix} \nabla^2 u \\ \nabla^2 v \end{bmatrix} ; |\alpha| \le 1;\ 0<\alpha^2 + \delta_1\delta_2 \le 1. \tag{1.1}$$

Any two-component system with constant diffusion matrix possessing real, nonnegative eigenvalues and nonnegative diagonal entries can be placed in the form of (1.1) by rescaling the space variables; the condition on $\alpha^2 + \delta_1\delta_2$ is equivalent to real, nonnegative eigenvalues for the matrix. The reason for this choice of diagonal coefficients is given below. The kinetic equations are assumed to possess an (exponentially) stable limit cycle $(U(t), V(t))$ with period T; the point $(U(0), V(0))$ is also assumed given so that $U(t)$, $V(t)$ has a unique meaning.

The limit cycle is a spatially homogeneous, oscillatory solution of the reaction-diffusion system (1.1). The linear stability problem for this solution is formulated by substituting $u = U(t) + \epsilon\hat{u}$, $v = V(t) + \epsilon\hat{v}$ into (1.1) to obtain the linear variational equation

$$\begin{bmatrix} \hat{u}_t \\ \hat{v}_t \end{bmatrix} = \begin{bmatrix} F_u(U(t), V(t)) & F_v(U(t), V(t)) \\ G_u(U(t), V(t)) & G_v(U(t), V(t)) \end{bmatrix} \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix} + \begin{bmatrix} 1+\alpha & \delta_2 \\ \delta_1 & 1-\alpha \end{bmatrix} \begin{bmatrix} \nabla^2 u \\ \nabla^2 v \end{bmatrix} . \tag{1.2}$$

Separating variables (or Fourier transforming) by $\hat{u} = p(t) \exp(-i \underset{\sim}{k} \cdot \underset{\sim}{x})$, $\hat{v} = q(t) \exp(-i \underset{\sim}{k} \cdot \underset{\sim}{x})$ yields the Floquet system (with the obvious definitions of $F_i(t)$, $G_i(t)$ as T-periodic functions)

$$\begin{bmatrix} p' \\ q' \end{bmatrix} = \begin{bmatrix} F_1(t) - (1+\alpha)k^2 & F_2(t) - \delta_2 k^2 \\ G_1(t) - \delta_1 k^2 & G_2(t) - (1-\alpha)k^2 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} ; \quad |\alpha| \le 1; \quad 0 \le \alpha^2 + \delta_1 \delta_2 \le 1. \tag{1.3}$$

The limit cycle is linearly unstable for wave number k^2 as a solution of the original system (1.1) iff (1.3) has an exponentially growing solution for that value k^2.

This chapter studies the linear stability of the limit cycle solutions to (1.1). Kopell and Howard (1973) and Othmer (1977) have mentioned the scarcity of results in this area, which seems a natural next step after stability studies of the spatially homogeneous, stationary solutions corresponding to critical points of the kinetic equations.

The stability of the stationary solutions was first considered by Turing (1952), who was the first to observe that a stable critical point of the kinetic system could be unstable when considered as a solution of the reaction-diffusion system. Specifically, he gave examples with the stationary state linearly stable to perturbations with small and large wave numbers k^2, but unstable to intermediate k^2. His work, together with subsequent work on the stability of stationary states, has been discussed in some detail in Chapter I.

The linear stability problem for spatially homogeneous, stationary states is fully solvable for a <u>given</u> system because the linearized equations have constant coefficients, i.e., the system corresponding to (1.3) has constant terms in place of the $F_i(t)$, $G_i(t)$, and the full solution can be written in terms of the coefficient matrix. (The <u>general</u> classification of behavior, however, is still quite complicated--see Othmer and Scriven (1969).) For spatially homogeneous oscillatory states the linear stability analysis yields the Floquet system (1.3) and no such general solution is possible.

The problem has attracted some attention, however. Kopell and Howard (1973) showed the limit cycle to remain linearly stable as a solution of the reaction-diffusion system when the diffusion matrix is scalar. Othmer (1977) considered the linear stability of the limit cycle solution on a finite domain with Neumann boundary conditions.

interpreted in our context of a spatially periodic perturbation, he showed the limit cycle to be stable to all large wave numbers k^2 and gave a sufficient condition for the linear stability of the limit cycle to perturbations for all wave numbers k^2 (see below). Conway, Hoff, and Smoller (1978) proved, under a basic assumption of a positively-invariant region for the solutions of the reaction-diffusion system, that solutions on finite spatial regions with Neumann boundary conditions decay to spatially homogeneous solutions of the kinetic equations if the regions are sufficiently small. (Their work deals with the solutions of the fully nonlinear system and not a linearized simplification.) For spatially periodic perturbations, their work also shows the limit cycle solution of (1.1) is stable to perturbations for all large wave numbers k^2 ($1/k^2$ corresponds to the size of the region). Cohen (1973) gave a singular perturbation approach for a class of reaction-diffusion equations of the form (1.1) arising in chemical reactor theory. These equations are on a finite spatial domain with particular boundary conditions and with diffusion coefficients $O(1/\epsilon)$, ϵ small. His calculations show that, in a time interval of $O(\epsilon)$, solutions decay to the spatially homogeneous limit cycle. Roughly speaking, this result corresponds to saying the limit cycle is stable to perturbations with large wave number $k^2 \sim 1/\epsilon$.

All these results require at least a nonsingular diffusion matrix, refer only to perturbations analogous to large wave numbers k^2, and show stability only. In this chapter stability for small wave numbers k^2 is studied, as well as for large wave numbers k^2 in the case of a singular diffusion matrix, and examples of limit cycles which are unstable--as solutions of the reaction-diffusion system--to small wave numbers k^2 are given.

This section closes with a direct proof that the limit cycle is linearly stable, as a solution to (1.1) with nonsingular diffusion matrix, to perturbations with large wave number k^2. A partial classification of the Floquet multipliers for (1.3), similar to that for Hill's equation (see Eastham, 1973, Chapter 1), is also given.

The second section gives a perturbation expansion calculating the Floquet exponents for (1.3) for small k^2, consequently determining linear stability of the limit cycle as a solution of (1.1). A simple characterization is obtained for stability and explicitly solvable examples are studied.

The third section constructs examples of the form (1.1) with limit cycles which are linearly unstable for small k^2 perturbations. Numerical results are presented in the fourth section pertaining to the examples of these unstable limit cycles. The numerical method used is Lees' Method for parabolic equations; it is discussed in detail, together with the program used, in Chapter V.

The fifth section uses a modification of a perturbation method for systems of differential equations with a large parameter (Coddington and Levinson, 1955, Chapter 6) to characterize linear stability of the limit cycle to large wave numbers k^2 . An advantage of this approach over others in the literature is its handling of singular diffusion matrices. Examples are studied.

The characterization of limit cycle stability to small k^2 also occurs in the multi-scaling method for perturbing the limit cycle studied in Chapter IV. The derivation of this one characterization by two completely different approaches and all the material of this chapter are from Cope (1979), which also contains some minor results, omitted here, on the linear stability of the limit cycle to intermediate wave numbers--a very intriguing open problem.

To see that (1.3) has only exponentially decaying solutions for large k^2 and a nonsingular diffusion matrix, set

$$\hat{\sigma} = \max_{[0,T]} \left(\text{spectral radius of } \begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \right)$$

$$\omega = \text{smaller eigenvalue of } \begin{bmatrix} 1+\alpha & \delta_2 \\ \delta_1 & 1-\alpha \end{bmatrix} > 0.$$

Then from (1.3) follows

$$\frac{1}{2}\,\frac{d}{dt}\,(p^2+q^2) \leq (\hat{\sigma}-\omega k^2)\,(p^2+q^2) \quad ,$$

forcing exponentially decaying solutions for $k^2 > \hat{\sigma}/\omega$. (This calculation fails when the diffusion matrix is singular, another example of the essential difference between the cases of singular and nonsingular diffusion matrices mentioned in Chapter I.) So the limit cycle is linearly stable as a solution of (1.1) to all large wave numbers k^2 if the diffusion matrix is nonsingular.

Othmer (1977) gave a sufficient condition for stability to all wave numbers k^2. His result is for general n-compo[illegible] preted for the case of (1.1) with $\delta_1 = \delta_2 = 0$, it says the limit cycle is linearly stable as a solution of (1.1) if

$$\frac{M-1}{M} \leq \frac{1+\alpha}{1-\alpha} \leq \frac{M}{M-1} \ ,$$

$$\text{where } M = \max_{[0,T]} \ ||\Theta^{-1}(t)|| \ ||\Theta(t)||$$

Here $\Theta(t)$ is any fundamental matrix for (1.3) with $k^2 = 0$ (Lemma C); $||\Theta(t)||$ means Euclidean norm. The result basically says that if the diffusion matrix is sufficiently close to the identity, the limit cycle is stable.

In the following, the fundamental matrix of (1.3) for $k^2 = 0$ is taken as known, namely,

$$\begin{bmatrix} U'(t) & \exp(-\mu t)\,\hat{U}(t) \\ V'(t) & \exp(-\mu t)\,\hat{V}(t) \end{bmatrix} ,$$

U', V' (derivatives of the limit cycle) and $\hat{U}$, $\hat{V}$ are [illegible] tions as in Lemma C in Appendix 1. Lemma C, of course, shows [illegible] fundamental matrix can be calculated from the limit cycle by single quadrature.

The choice of $1 \pm \alpha$ as a normalized form for the diagonal diffusion coefficients in (1.1) was deliberate - a simplification of the behavior of the Floquet multipliers in (1.3) results. Set

$$\begin{bmatrix} p \\ \\ q \end{bmatrix} = \exp(-k^2 t) \begin{bmatrix} x \\ \\ y \end{bmatrix} , \qquad (1.5a)$$

so (1.3) becomes

$$\begin{bmatrix} x' \\ \\ y' \end{bmatrix} = \begin{bmatrix} F_1(t) - \alpha k^2 & F_2(t) - \delta_2 k^2 \\ \\ G_1(t) - \delta_1 k^2 & G_2(t) + \alpha k^2 \end{bmatrix} \begin{bmatrix} x \\ \\ y \end{bmatrix} , \qquad (1.5b)$$

and note that (1.3) has exponentially increasing solutions iff (1.5b) has solutions with growth rate greater than $\exp(+k^2 t)$.

Define the fundamental matrix

$$X(t) = \begin{bmatrix} x_1(t) & x_2(t) \\ \\ y_1(t) & y_2(t) \end{bmatrix}, \quad X(0) = \text{identity}$$

The Floquet multipliers ρ_1, ρ_2 are the eigenvalues of X(T) (Eastham, 1977, Chapter 1), and they determine the exponential growth of the solution: if $\rho_i = \exp(-\mu_i T)$, then the solutions of (1.5b) grow like $\exp(-\mu_i t)$. Consequently,

$$\rho^2 - [x_1(T) + y_2(T)]\rho + [x_1(T)y_2(T) - x_2(T)y_1(T)] = 0, \qquad (1.6)$$

equivalently, $\rho^2 - D(k^2)\rho + \exp(-\mu T) = 0$.

The last term $\exp(-\mu T)$ follows from using Lemma B.2 (Abel's Identity) to evaluate the determinant, noting that the trace of the coefficient matrix in (1.4b) is independent of k^2, and at $k^2 = 0$ the determinant is $\exp(-\mu T)$ (product of the Floquet multipliers 1 and $\exp(-\mu T)$). The two Floquet multipliers for (1.5b) are therefore determined by a single quantity $D(k^2)$, the <u>discriminant</u> in the terminology of Hill's equation, and a description of the behavior of the multipliers can be given by breaking down the possibilities for $D(k^2)$:

$$\begin{array}{lll}
\text{(a)} & |D(k^2)| > 2\exp(-\frac{\mu}{2}T). & \text{The roots are real and both have the same sign as } D\,. \\
\text{(b)} & |D(k^2)| = 2\exp(-\frac{\mu}{2}T). & \text{Both roots} = \exp(-\frac{\mu}{2}T)\text{, or both} = -\exp(-\frac{\mu}{2}T)\,. \\
\text{(c)} & |D(k^2)| < 2\exp(-\frac{\mu}{2}T). & \text{Both roots are complex conjugate and have modulus } \exp(-\frac{\mu}{2}T).
\end{array} \tag{1.7}$$

At $k^2 = 0$, the roots are 1 and $\exp(-\mu T)$, so case (a) holds. As k^2 increases, the two roots may go further apart (both necessarily remaining positive) or come together at $\exp(-\frac{\mu}{2}T)$. They may either cross at $\exp(-\frac{\mu}{2}T)$ or split into the complex plane, remaining on the circle of radius $\exp(-\frac{\mu}{2}T)$. They may reach the negative real axis on this circle or return to the positive real axis.

In particular, a linearly unstable limit cycle, which can occur only when some $|\rho_i| > \exp(k^2 T)$, can only occur for two real Floquet multipliers.

A Perturbation Expansion for Small Wave Numbers k^2

Since the solution of (1.3) is known for $k^2 = 0$, it is natural to try an expansion in powers of k^2. For $k^2 = 0$ in (1.3), one solution decays like exp $(-\mu t)$ and it is unlikely to be perturbed to a growing solution, so we consider the other periodic solution. It may be perturbed by $O(k^2)$ - terms to a growth rate like exp $(Bk^2 t)$, which will grow or decay depenuing on the sign of B. The Floquet representation suggests a solution of (1.3) of the form

$$\begin{bmatrix} p \\ q \end{bmatrix} = \exp\left(\left(\sum_{n=1}^{\infty} B_n \, k^{2n}\right) t\right) \sum_{n=0}^{\infty} \begin{bmatrix} p_n(t) \\ q_n(t) \end{bmatrix} k^{2n} \quad , \qquad (2.1)$$

where $\begin{bmatrix} p_n(t) \\ q_n(t) \end{bmatrix}$ are T - periodic functions and $\begin{bmatrix} p_o(t) \\ q_o(t) \end{bmatrix} = \begin{bmatrix} U'(t) \\ V'(t) \end{bmatrix}$.

Substitution into (1.3) yields as the coefficient of k^{2n}, $n \geq 1$,

$$\begin{bmatrix} p_n' \\ q_n' \end{bmatrix} = \begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \begin{bmatrix} p_n \\ q_n \end{bmatrix} - \begin{bmatrix} 1+\alpha & \delta_2 \\ \delta_1 & 1-\alpha \end{bmatrix} \begin{bmatrix} p_{n-1} \\ q_{n-1} \end{bmatrix} - \sum_{m=1}^{n} B_m \begin{bmatrix} p_{n-m} \\ q_{n-m} \end{bmatrix} \qquad (2.2)$$

For $n = 1$, the equation becomes

$$\begin{bmatrix} p'_1 \\ q'_1 \end{bmatrix} = \begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \begin{bmatrix} p_1 \\ q_1 \end{bmatrix} - \begin{bmatrix} 1 + \alpha & \delta_2 \\ \alpha_1 & 1 - \alpha \end{bmatrix} \begin{bmatrix} U' \\ V' \end{bmatrix} - \delta_1 \begin{bmatrix} U' \\ V' \end{bmatrix} \tag{2.3}$$

From Lemma D in Appendix I, this equation has a T-periodic solution iff

$$B_1 = \frac{-1}{T} \int_0^T \left(1 + \frac{\alpha(U'\hat{V} + V'\hat{U}) - \delta_1 U'\hat{U} + \delta_2 V'\hat{V}}{U'\hat{V} - V'\hat{U}} \right) ds, \tag{2.4}$$

$$= -1 + (A_0 \alpha + A_1 \delta_1 + A_2 \delta_2) \quad ,$$

where A_0, A_1, A_2 are the definite integrals forming the coefficients of α, δ_1, δ_2 .

Having determined B_1, Lemma D says the periodic solution p_1, q_1 is determined up to an arbitrary constant. (One possible choice is to require p_n, q_n to satisfy

$$\int_0^T (p_n U' + q_n V')\, dt = 0 \text{ for } n \geq 1 .)$$

Notice the series is well defined to all orders – the only unknown is the coefficient of k^{2n} is B_n, which is determined uniquely by the condition that p_n, q_n be T-periodic, using Lemma D.

Summarizing (2.4) :

THEOREM 1. The limit cycle is linearly unstable as a solution of

(1.1) to small wave numbers k^2 iff $A_0\alpha + \delta_1 A_1 + \delta_2 A_2 > 1$ (as defined in (2.4).

In particular, if $\delta_1 = \delta_2 = 0$, the limit cycle is unstable for all small k^2 if $A_0 > 1$. It may seem to violate continuity for the limit cycle to be stable at $k^2 = 0$ and unstable for all small $k^2 > 0$. However, an analogous case occurs for critical points: if the (kinetically) stable critical point has eigenvalues 0 , $-\mu$ with respect to the kinetic equation, then the constant solution corresponding to the 0-eigenvalue can be made unstable by the addition of diffusion terms. The (kinetically) stable limit cycle has Floquet exponents 0 , $-\mu$ with respect to the kinetic equation and the periodic solution corresponding to the 0-Floquet exponent can be made unstable by the diffusion terms.

As examples, we consider two classes of equations for which the limit cycle and related functions can be calculated explicitly.

Let (1.1) be a λ-ω system with full diffusion matrix ($R^2 = u^2 + v^2$):

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} \lambda(R) & -\omega(R) \\ \omega(R) & \lambda(R) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} (1+\alpha) & \delta_2 \\ \delta_1 & (1-\alpha) \end{bmatrix} \begin{bmatrix} \nabla^2 u \\ \nabla^2 v \end{bmatrix} ; \tag{2.5}$$

$$|\alpha| \le 1; \quad 0 \le \alpha^2 + \delta_1 \delta_2 \le 1 \quad .$$

The kinetic equations have the limit cycle solution $U(t) = R_0 \cos(\omega_0 t)$, $V(t) = R_0 \sin(\omega_0 t)$, with $\lambda(R_0) = 0$, $\omega_0 = \omega(R_0)$. The analogue of (1.3) is

$$\begin{bmatrix} p' \\ q' \end{bmatrix} = \begin{bmatrix} R_0S_0\cos(\omega_0 t)\cos(\omega_0 t+\sigma_0)-k^2(1+\alpha) & R_0S_0\sin(\omega_0 t)\cos(\omega_0 t+\sigma_0) -\omega_0-k^2\delta_2 \\ R_0S_0\cos(\omega_0 t)\sin(\omega_0 t+\sigma_0)+\omega_0-k^2\delta_1 & R_0S_0\sin(\omega_0 t)\sin(\omega_0 t+\sigma_0)-k^2(1-\alpha) \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix}, \tag{2.6}$$

where $S_0\cos\sigma_0 = \lambda'(R_0)$, $S_0\sin\sigma_0 = \omega'(R_0)$, $S_0 > 0$, and $-\mu = R_0\lambda'(R_0)$ with the assumption $-\mu < 0$ to insure stability of the limit cycle.

The fundamental matrix, found by Lemma C, is

$$\begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U}(t) \\ V'(t) & \exp(-\mu t)\hat{V}(t) \end{bmatrix} = \begin{bmatrix} -R_0\omega_0\sin(\omega_0 t) & -\exp(-\mu t)\dfrac{\cos(\omega_0 t+\sigma_0)}{R_0\omega_0\cos\sigma_0} \\ R_0\omega_0\cos(\omega_0 t) & -\exp(-\mu t)\dfrac{\sin(\omega_0 t+\sigma_0)}{R_0\omega_0\cos\sigma_0} \end{bmatrix} \tag{2.7}$$

Substitution into (2.4) gives:

(a) $A_0 = 0$; (2.8)

(b) $A_1 = -\frac{1}{2}\tan\sigma_0$;

(c) $A_2 = \frac{1}{2}\tan\sigma_0$.

In Theorem 1, therefore, $A_0\alpha + A_1\delta_1 + A_2\delta_2 = \frac{1}{2}(\delta_2-\delta_1)\tan\sigma_0$. In particular, for $\delta_1 = \delta_2 = 0$, the limit cycle of <u>any</u> $\lambda-\omega$ system (2.5) is linearly stable to perturbations for small wave numbers k^2 since $|A_0| = 0 < 1$.

Next, consider the system

$$\begin{bmatrix} u_t \\ \\ v_t \end{bmatrix} = \begin{bmatrix} a(1-u^2)u-v \\ \\ u+a(1-bu^2)v \end{bmatrix} + \begin{bmatrix} (1+\alpha)\nabla^2 u \\ \\ (1-\alpha)\nabla^2 v \end{bmatrix} \quad ; \quad |\alpha| \le 1 \; ; \; a,b > 0 \; . \tag{2.9}$$

This system occurs as a model in the study of chemical reactors (Cohen (1973) and Cohen, Hoppensteadt, and Miura (1977) - (2.9) is a rescaled form of equations in these papers). We have found an exact solution in the case b = +1, used here as a second sample.

The substitution $u = R\cos\psi$, $v = R\sin\psi$ changes the kinetic equations of (2.9) to

$$\begin{aligned} R' &= aR(1 - (R\cos\psi)^2) + a(1-b)R^3(\cos\psi\sin\psi)^2 \\ \psi' &= 1 + a(1-b)R^2(\cos\psi)^3\sin\psi \quad . \end{aligned} \tag{2.10}$$

For $\underline{b = +1}$, these equations reduce to a Bernoulli equation for R with solution

$$\begin{aligned} \frac{1}{R^2} &= \frac{1}{2} + \frac{1}{2}\;\frac{a^2\cos 2\psi + a\sin 2\psi}{a^2+1} + C_2\exp(-2a\psi) \\ \psi &= t + C_1 \quad . \end{aligned} \tag{2.11}$$

Setting $C_1, C_2 = 0$ gives the limit cycle $(U(t), V(t)) = (R_0(t)\cos t, R_0(t)\sin t)$, and the analogue of (1.3) is

$$\begin{bmatrix} p' \\ q' \end{bmatrix} = \begin{bmatrix} a(1-3U^2)-k^2(1+\alpha) & -1 \\ 1-2aUV & a(1-U^2)-k^2(1-\alpha) \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} . \tag{2.12}$$

The fundamental matrix for $k^2 = 0$ is

$$\begin{bmatrix} U'(t) & \exp(-2at)\hat{U}(t) \\ V'(t) & \exp(-2at)\hat{V}(t) \end{bmatrix} = \begin{bmatrix} R_0' \cos t - R_0 \sin t & \exp(-2at)R_0^3 \cos t \\ R_0' \sin t + R_0 \cos t & \exp(-2at)R_0^3 \sin t \end{bmatrix} . \tag{2.13}$$

(Incidentally, since the full solution is known, the easiest way to obtain the second solution is to differentiate (2.11) with respect to C_2 at $C_2 = 0$, as suggested in Lefschetz, 1977, Chapter 3.)

The Wronskian of (2.13) is $-\exp(-2at)R_0^4$, and (2.4) gives

$$A_0 = \frac{1}{2\pi} \int_0^{2\pi} \frac{a^2+(a^2+1)\cos 2t}{a^2+1+a^2 \cos 2t + a\sin 2t} \, dt . \tag{2.14}$$

The integral can be evaluated by the substitution $z = \exp(+it)$, giving

$$A_0 = \frac{1}{2\pi} \oint_{|z|=1} \frac{(a^2+1)z^4+2a^2z^2+(a^2+1)}{(a^2-ai)z^4+2(a^2+1)z^2+(a^2+ia)} \, \frac{dz}{iz} .$$

The denominator has roots at

$$z^2 = \frac{1}{a^2-ai}\left[-(a^2+1) \pm (a^2+1)^{1/2}\right] ,$$

with one pair inside the unit circle and one pair outside for all $0 < a < +\infty$. Evaluating the residues at $z = 0$ and at the pair of roots inside the unit circle gives

$$A_0 = \frac{(a^2+1)^{1/2}-1}{(a^2+1)^{1/2}} \quad , \quad 0 < a < +\infty . \tag{2.15}$$

Since $0 < A_0 < 1$ for all $a > 0$, Theorem 1 shows the limit cycles of (2.9) (with $b = 1$) to be stable to perturbations of small wave numbers k^2 for all α, $|\alpha| \leq 1$.

These examples show only stable behavior when the diffusion matrix is diagonal. Explicitly solvable examples of systems with diagonal diffusion matrices showing unstable behavior will be constructed in the next section.

Explicit Examples of Instability for Small k^2

In this section we construct examples of explicitly solvable systems of the form (1.1) with cross terms $\delta_1 = \delta_2 = 0$ for which $|A_0| > 1$ (A_0 defined in (2.4)). By Theorem 1, it follows that as the parameter α in the diffusion matrix varies past $1/A_0$, the limit cycle suddenly switches from being stable to being unstable for all perturbations of small wave numbers k^2. A numerical examination of this behavior is given in the last section of this chapter.

We wish to construct examples of (1.1) with diagonal diffusion matrix such that (a) the limit cycle and associated functions can be found explicitly, (b) A_0 can be evaluated explicitly, and (c) $|A_0| > 1$. As shown in the second section, all $\lambda - \omega$ systems have $A_0 = 0$. Also, the explicitly solvable case of (2.9) has $0 < A_o < 1$ for all values of the parameter a. This difficulty in finding suitable examples is overcome by the following systematic procedure:

(1) Consider systems (1.1) with <u>almost</u> solvable kinetic equations: see (3.1);

(2) for kinetic equations of the form (3.1), the value of A_0 can be written in a simplified form: see Lemma 1;

(3) to make the equations more nearly solvable a further restriction is made: see (3.6);

(4) under the new restriction, Lemma 1 simplifies further: see (3.9);

(5) finally, the expression for A_0 in (3.9) is sufficiently simple that explicitly solvable examples with $|A_0| > 1$ can be constructed by guessing.

To begin, notice that the kinetic equations of (1.1) are reduced by the substitution $u = R\cos\psi$, $v = R\sin\psi$ to

$$\begin{bmatrix} R' \\ \psi' \end{bmatrix} = \begin{bmatrix} u/R & v/R \\ -v/R^2 & u/R^2 \end{bmatrix} \begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} = \begin{bmatrix} R\lambda(R,\psi) \\ \omega(R,\psi) \end{bmatrix} ,$$

where prime $'$ means derivative with respect to t and λ,ω are 2π-periodic functions of ψ. First restrict attention to kinetic equations with the polar form:

$$\text{(a)}\quad R' = R\lambda(R), \qquad (3.1)$$
$$\psi' = \omega(R,\psi);$$
$$\text{(b)}\quad \lambda(R_0) = 0 \text{ for some } R_0 > 0 \text{ and } \lambda_R(R_0) < 0 ;$$
$$\text{(c)}\quad \omega(R_0,\psi) > 0 \text{ for all } \psi ;$$
$$\text{(d)}\quad \omega(R,\psi+2\pi) = \omega(R,\psi) .$$

Conditions (a), (b), and (c) say that $R = R_0$ is a stable limit cycle and (d) is the obvious periodicity required of a polar transformation. This is step (1).

To calculate A_0, the limit cycle and the solution of the variational equation must be known. The limit cycle is $(U,V) = (R_0\cos(\psi_0(t)), R_0\sin(\psi_0(t))$, where

$$\text{(a)}\quad \psi_0' = \omega(R_0, \psi_0) \text{ with } \psi_0(0) = 0 , \qquad (3.2)$$

$$\text{(b)}\quad T = \int_0^{2\pi} \frac{d\psi}{\omega(R_0,\psi)} .$$

It is convenient to retain the polar form for finding solutions of the variational equations. Setting $R = R_0 + \epsilon\rho$, $\psi = \psi_0 + \epsilon\phi$ in (3.1a) (corresponding to $u + \epsilon(\rho\cos\psi_0 - R_0\sin\psi_0\phi$, $v + \epsilon(\rho\sin\psi_0 + R_0\cos\psi_0\phi))$ leads to the variational equations

$$\rho' = R_0\lambda_R(R_0)\rho \ , \tag{3.3}$$

$$\phi' = \omega_R(R_0,\psi_0)\rho + \omega_\psi(R_0,\psi_0)\phi \ .$$

One solution is clearly $\rho = 0$, $\phi = \psi_0'$, corresponding to the periodic solution (U', V'). Setting $-\mu = R_0\lambda_R(R_0)$ and $\rho(0) = 1$, a second solution for ρ is $\rho = \exp(-\mu t)$. To obtain ϕ, a convenient substitution is $\phi = \exp(-\mu t)\psi_0'\theta$; using (3.2a), the equation for θ reduces to

$$\theta' - \mu\theta = \frac{\omega_R(R_0,\psi_0)}{\omega(R_0,\psi_0)} \ , \tag{3.4a}$$

and the desired solution is the unique T-periodic solution (see Lemma A in Appendix I). Actually, θ as a function of ψ will be more useful, so that $\theta(\psi)$ is the unique 2π-periodic solution to

$$\frac{d\theta}{d\psi} - \frac{\mu}{\omega(R_0,\psi)}\theta = \frac{\omega_R(R_0,\psi)}{(\omega(R_0,\psi))^2} \ . \tag{3.4b}$$

The solutions to the variational equation can now be written as

$$\begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U}(t) \\ V'(t) & \exp(-\mu t)\hat{V}(t) \end{bmatrix} = \begin{bmatrix} -R_0\sin\psi_0\psi_0' & \exp(-\mu t)(\cos\psi_0 - R_0\sin\psi_0\psi_0') \\ R_0\cos\psi_0\psi_0' & \exp(-\mu t)(\sin\psi_0 + R_0\cos\psi_0\psi_0') \end{bmatrix}$$

Substitution of these expressions into (2.4) yields an expression for A_0. Summarizing to finish Step 2:

Lemma 1. For the system (1.1) with kinetic equations (in polar form) given by (3.1),

$$A_0 = \frac{1}{T}\int_0^T [\cos(2\psi_0(t) - R_0\sin(2\psi_0(t))\psi_0'(t)\theta(t)]dt$$

$$= \frac{1}{T}\int_0^{2\pi} [\frac{\cos(2\psi)}{\omega(R_0,\psi)} - R_0\sin(2\psi)\theta(\psi)]\, d\psi \quad ,$$

where $\psi_0(t),T$ are given by (3.2) and $\Theta(t)$ (or $\Theta(\psi)$) is the unique T-periodic (or 2π-periodic) solution to (3.4).

We now try to pick $\omega(R,\psi)$ so that ψ_0 and θ can be found. Some experimentation suggests the additional constraint (n = arbitrary constant)

(a) $$\frac{1}{\omega(R,\psi)} = \frac{h(R)}{\mu}\left[-n\frac{f'(\psi)}{f(\psi)} + g(R)\right]; \qquad (3.6)$$

(b) $f(\psi)$ is positive and 2π-periodic;

(c) $h(R_0) = +1$ and $g(R)$ is such that $\omega(R,\psi) > 0$ for all $R > 0$ and all ψ.

(Although $\omega(R_0,\psi) > 0$ is sufficient, (3.6c) is chosen to give a simpler phase plane - the origin is the only possible critical point.) Such an ω is still sufficiently general that some choice of f, g, h can be expected to force $|A_0| > 1$. This ends Step 3.

The restrictions (3.6) give simple expressions for ψ_0, θ.

Substitution into (3.2) gives

(3.7)

$$\text{(a)} \quad t(\psi) = \frac{1}{\mu}\left[g(R_0)\psi - n \ln \frac{f(\psi)}{f(0)}\right] \quad \text{defining} \quad \psi_0(t) \quad ;$$

$$\text{(b)} \quad T = 2\pi \frac{g(R_0)}{\mu} \quad .$$

Substitution into (3.4b) gives

(3.8)

$$\text{(a)} \quad \theta(\psi) = \frac{1}{\mu}\left[- F(R_0,\psi)\ g'(R_0)\ (f(\psi))^{-n} + h'\ (R_0)\right]$$

where $F(R_0,\psi)$ is the unique periodic (in ψ) function (Lemma A.2) defined by

(3.8)

$$\text{(b)} \quad F(R_0,\psi) = \exp(g(R_0)\psi)[C(R_0) + \int_0^{\psi} \exp(-g(R_0)s)(f(s))^n ds].$$

Therefore, assuming $\omega(R,\psi)$ is given by (3.6) and substituting (3.6) - (3.8) into Lemma 1 yields

$$A_0 = \frac{1}{2\pi g(R_0)} \int_0^{2\pi} [-n \cos(2\psi) \frac{f'(\psi)}{f(\psi)} \tag{3.9}$$

$$+ R_0 g'(R_0)\sin(2\psi)(f(\psi))^{-n} F(R_0,\psi)]d\psi .$$

This finishes Step (4).

Although the expression for A_0 would simplify considerably if we required $g'(R_0) = 0$, this will not give the desired examples because $|A_0| < 1$: since $\omega(R_0,\psi) > 0$, clearly

AD-A087 114 CENTER FOR NAVAL ANALYSES ALEXANDRIA VA OPERATIONS EV--ETC F/G 7/4
LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS.(U)
JUN 80 D COPE
UNCLASSIFIED OEG-PP-287 NL

2 OF 4
AD A
087114

$$\int_0^{2\pi} \cos(2\psi) \frac{d\psi}{\omega(R_0,\psi)} < \int_0^{2\pi} \frac{d\psi}{\omega(R_0,\psi)} .$$

The integral on the right is $2\pi g(R_0)/\mu$. Substituting (3.6a) into the integral on the right and assuming $g'(R_0) = 0$ in (3.9), the left side becomes $(2\pi g(R_0)/\mu)\ |A_0|$, or $|A_0| < 1$.

We are now ready to carry out Step (5). Explicit choices will be made for $n, h(R)$, $f(\psi)$ and the appropriate conditions on $g(R)$ deduced.

(3.10)

(a) $n = +1;\ h(R) = +1;\ f(\psi) = 1 + \epsilon\cos 2\psi$ with $|\epsilon| < 1$.

Since

$$\max \left| \frac{f'(\psi)}{f(\psi)} \right| = \max \left| \frac{2\epsilon \sin 2\psi}{1 + \epsilon \cos 2\psi} \right| = \frac{2|\epsilon|}{(1-\epsilon^2)^{1/2}} ,$$

(3.6c) can be satisfied by

(3.10)

(b) $g(R) > \dfrac{2|\epsilon|}{(1-\epsilon^2)^{1/2}}$ for all R.

Calculation of $F(R_0,\psi)$ and substitution into (3.9) gives

$$A_0 = \frac{1}{2\pi g(R_0)} \int_0^{2\pi} \left\{ \frac{-2\epsilon \cos 2\psi \sin 2\psi}{1+\epsilon\cos 2\psi} + \frac{R_0 g'(R_0) \sin 2\psi}{1+\epsilon \cos 2\psi} \left[-\frac{1}{g(R_0)} + \frac{\epsilon(-g(R_0)\cos 2\psi + 2\sin 2\psi)}{(g(R_0))^2 + 4} \right] \right\} d\psi .$$

This integral simplifies, due to perfect derivatives, to

$$A_0 = \frac{R_0 g'(R_0)\epsilon}{\pi g(R_0)[(g(R_0))^2 + 4]} \int_0^{2\pi} \frac{(\sin 2\psi)^2 d\psi}{1 + \epsilon \cos 2\psi} .$$

The substitution $z = \exp(+i\psi)$ and use of the Residue Theorem gives

$$\text{(c)} \quad A_0 = \frac{2R_0}{\epsilon} \left[1 - (1-\epsilon^2)^{1/2}\right] \frac{g'(R_0)}{g(R_0)[g(R_0))^2 + 4]} \quad . \qquad (3.10)$$

Therefore, <u>for each ϵ , $0 < |\epsilon| < 1$, any function $g(R)$ with $1 < |A_0|$ in (3.10c) and satisfying (3.10b) can be used to construct an example of (1.1) with limit cycle unstable to small wave numbers k^2 .</u> The kinetic equations are constructed using (3.1a), (3.6a), and (3.10 a,b,c), in which case all other conditions (3.1 b,c,d), (3.6 b,c) are automatically satisfied. Instability occurs as α varies past $1/A_0$, $|\alpha|$ increasing.

A specific system, constructed according to this prescription, is studied numerically in the next section of this chapter.

Numerical Results for an Unstable Limit Cycle

In the previous section, examples of (1.1) with diagonal diffusion matrices were constructed whose limit cycles become linearly unstable to all small wave numbers k^2 as the diffusion parameter passes a critical value α_0. The linear analysis gives $\alpha_0 = 1/A_0 + O(k^2)$. In this section a specific example of such a system is selected and small wave number perturbations of the limit cycle are examined numerically for various values of α.

First, following the instructions at the end of the previous section, the kinetic system of (1.1) is assumed to have the polar form

$$R' = R(1-R^2) \quad , \tag{4.1)(a}$$

$$\psi' = \omega(R,\psi) \quad \text{with} \quad \frac{1}{\omega(R,\psi)} = \frac{3\sin 2\psi}{5 + 3\cos 2\psi} + \frac{1}{2}\, g(R) \quad .$$

This choice satisfies (3.1a) with limit cycle radius $R_0 = 1$ and Floquet exponent $-\mu = + R_0\lambda'(R_0) = -2$, and satisfies (3.6a), (3.10a) with $\epsilon = \frac{3}{5}$. We choose

$$g(R) = \frac{11}{4} + \tanh(a(R^2-1)) \quad , \tag{4.1)(b}$$

which satisfies the lower bound of (3.10b) with $\epsilon = \frac{3}{5}$. From (3.10c) follows

$$A_0 = \frac{256a}{6105} = .0419a \quad . \tag{4.1)(c}$$

The limit cycle period is (from (3.2b))

$$T = \frac{11\pi}{4} = 8.64 \quad . \tag{4.1)(d}$$

In terms of the original variables, the system under (4.2) consideration is

$$u_t = u(1-u^2-v^2) - v\omega + (1+\alpha)u_{xx},$$

$$v_t = v(1-u^2-v^2) + u\omega + (1-\alpha)v_{xx} \quad ,$$

$$\text{where } \omega = \frac{8u^2 + 2v^2}{6uv + (4u^2+v^2)\left(\frac{11}{4} + \tanh(a(u^2+v^2-1))\right)} \quad .$$

For $a > 0$, the limit cycle should go unstable to all small wave numbers k^2 as α increase past $\alpha_0 \sim 1/A_0 = 23.9/a$. The large value of a required to make $\alpha_0 < 1$ makes ω nearly discontinuous across the limit cycle.

Lees' method (Lees 1969, Varah 1978) was used for the numerical solution of (4.2). This difference scheme is an extrapolated variation of the Crank-Nicolson method; it will be discussed in more detail in Chapter V. Lees' method is easily programmed, has accuracy $O((\Delta x)^2 + (\Delta t)^2)$ and is stable. (In the actual implementation of the program, initial data and the diffusion coefficients were rescaled to obtain the equivalent system for the fixed interval $0 \leq x \leq 1$; the step sizes were
$\Delta x = .02$ and $\Delta t = T/500 \sim .017$)

It is useful to consider the spatially periodic solutions as time dependent curves in the phase plane. For periodic boundary conditions, $(u(x,t), v(x,t))$ at each value of t is a closed curve. A perturbation of the limit cycle at $t = 0$ corresponds to a small closed curve near some point on the limit cycle - for instance, the initial data of our computer runs (before scaling to $0 \leq x \leq 1$) consisted of

$$u(x,0) = 1 \tag{4.3}$$
$$v(x,0) = .1 \cos(.2x),$$

corresponding to wave number $k^2 = .04$. To represent the results of the calculations, polar coordinates are especially useful: for $u = R\cos\psi$, $v = R\sin\psi$, define

$$\Delta R = \max_x R(x,t) - \min_x R(x,t) \quad ,$$

$$\Delta\psi = \max_x \quad (x,t) - \min_x \quad (x,t) \quad .$$

These two quantities give a t-dependent annular segment in which the solution lies. For example, the initial data (4.3) gives $\Delta R \sim .005$ and $\Delta\psi \sim .2$ at $t = 0$.

One expects that $\Delta R, \Delta\psi \to 0$ as $t \to +\infty$ for a stable limit cycle and other behavior for an unstable one, but difficulties arise in attempting to observe this behavior. First, ΔR becomes very small (that is, $R(x,t) \sim 1$) in all computer runs, both for stable and unstable cases, and growth or decay is most easily observed in $\Delta\psi$. Two problems occur in observing $\Delta\psi$. From the second section, the growth (or decay) rate for the larger Floquet exponent is approximately $\exp((-1+A_0\alpha)k^2t)$. Using $k^2 = .04$ and (4.1c) with $a > 0$, the maximum growth rate occurs for $\alpha = +1$. This maximum is $\exp(.044t)$ for $a = 50$ (the value used in the calculations), a rather mild growth rate. To observe growth, then, one must integrate the equations over quite long time intervals. Furthermore, $\Delta\psi$ undergoes oscillations over each period of the limit cycle, typically varying by a factor of about 3 (for instance, for (4.2) with $a = 50$, initial data (4.3), and

$\alpha = .9$, $\Delta\psi$ varies between .085 and .230 on (0,T], between .079 and .215 on (T,2T], etc.) These fluctuations mean growth or decay cannot be determined by observing $\Delta\psi$ at some arbitrary sequence of times. As a measure of growth or decay, we give <u>maximum values of $\Delta\psi$</u> over the intervals (0,T], (T,2T], (2T,3T], etc. For $a = 50$ and various values of α , the successive maxima of $\Delta\psi$ are (see Figure 2 also):

$\alpha = .70$	.256,	.233,	.214,	.197,
	.182,	.168,	.156,	.145,
	.134,	.125,	.116,	.108,
$\alpha = .80$	.243,	.225,	.211,	.197,
	.184,	.173,	.162,	.151,
	.142,	.133,	.125,	.117.
$\alpha = .90$	.230,	.215,	.202,	.190,
	.176,	.169,	.427,	.598.
$\alpha = .99$	.218,	.204,	.330,	.527,
	.613,	.676,	.674,	.674.

Experimentation with different step sizes suggests the above values for $\Delta\psi$ are accurate. The linearized analysis shows instability for $.478 \leq \alpha \leq 1$. For $\alpha = .99$, growth begins to show at $t \sim 3T$; for $\alpha = .90$, at $t \sim 7T$. Presumably growth would appear for $\alpha = .80$ and

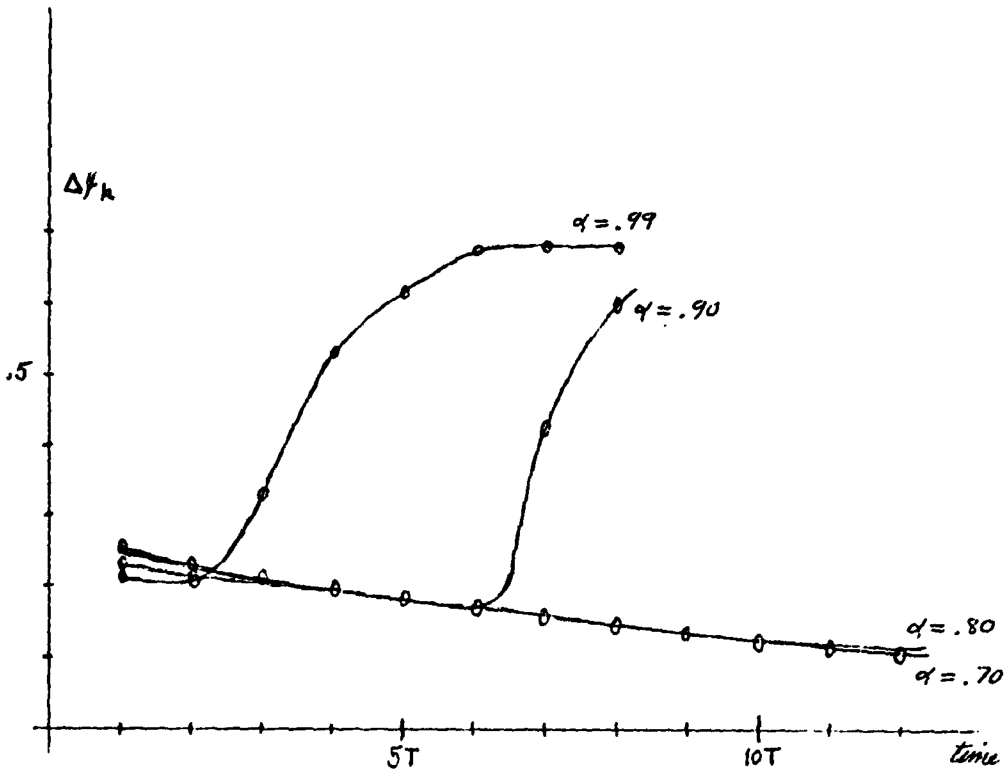


FIGURE 2. GRAPH OF

$$\Delta\psi_k = \max_{((k-1)T,\, kT]} \Delta\psi \ , \quad k = 1, 2, 3, \ldots,$$

SHOWING THE ONSET OF INSTABILITY (ONLY CIRCLES REPRESENT DATA - THE SMOOTH LINES ARE SIMPLY TO CONNECT CIRCLES FOR THE SAME VALUE OF α). THE LINEARIZED ANALYSIS SHOWS $\alpha = .80, .70$ TO BE UNSTABLE ALSO, AND PRESUMABLY THEY WOULD HAVE SHOWN GROWTH AT LARGER TIME VALUES.

.70 if the calculations had been extended beyond 12T.* (As mentioned above, the maximum growth rate here is exp (.044t) for $\alpha = 1$ and decreases with α .) Of course the data for $\alpha = .90$ and $= .99$ confirm that a (kinetically) stable limit cycle can become unstable as a solution of the fully nonlinear system.

The system (4.2) was also considered with $a = 30$, in which case the linearized result gives instability occurring for $\alpha_0 \sim 1/A_0 = .796$ using (4.1c)). However, numerical solutions for $\alpha = .999$, initial data (4.3), and $k^2 = .04$ show no instability. In this case the full nonlinearity appears to have completely damped out the linear growth.

*The time interval 12T is already 6000 time steps, and it is quite possible that the extremely slow growth of the instability is overwhelmed by numerical hash.

A Perturbation Expansion for Large Wave Numbers k^2

As $k^2 \to +\infty$ in (1.3), we obtain a system of differential equations containing a large parameter and a well-developed asymptotic theory exists. For instance, systems of the form (1.3) are treated in Chapter 6 of Coddington and Levinson (1955). Notice that the matrix coefficient of k^2 is

$$\begin{bmatrix} -(1+\alpha) & -\delta_2 \\ -\delta_1 & -(1-\alpha) \end{bmatrix} \text{ with eigenvalues } -1 \pm \delta, \quad \delta = (\alpha^2 + \delta_1\delta_2)^{1/2} . \tag{5.1a}$$

$$-1+\delta \text{ has the eigenvector } \begin{bmatrix} a \\ b \end{bmatrix}, \quad -1-\delta \text{ has } \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} \tag{5.1b}$$

If the eigenvalues are assumed distinct $(\delta \neq 0)$, then Theorem 2.1 of that chapter states that a fundamental matrix

$$P(k^2,t)\exp(k^2 Q_0(t) + Q_1(t))$$

can be formally constructed such that

$$P(k^2 t) = \sum_{n=0}^{\infty} k^{-2n} P_n(t) \text{ with each matrix } P_n(t) \text{ independent of } k^2, \tag{5.2a}$$

$$Q_0'(t) = \begin{bmatrix} -1+\delta & 0 \\ 0 & -1-\delta \end{bmatrix} \text{ and } Q_0(t),\ Q_1(t) \text{ are diagonal matrices.} \tag{5.2b}$$

Furthermore, Theorem 3.1 of that chapter also holds and the formal solution given by (4.2) on [0,T] is asymptotic to the real solution on [0,T] as $k^2 \to +\infty$.

As it stands, (5.2) is sufficient to give the desired leading order behavior. However, since it was derived for quite general systems, it does not represent the solution in Floquet normal form ($P(k^2,t)$ will not necessarily be periodic even for Floquet systems). We give here an alternate expansion, based on the Floquet representation, which yields another form of the solution.

Using the eigendata defined in (5.1), we show that the solution corresponding to the larger Floquet multiplier can be written as (assuming $\delta \neq 0$ to avoid a multiple eigenvalue):

$$\begin{bmatrix} p \\ \\ q \end{bmatrix} = \exp\left((-1+\delta)k^2 t + \sum_{n=0}^{\infty} k^{-2n} C_n(t)\right) \begin{bmatrix} a \\ \\ b \end{bmatrix} + \sum_{n=0}^{\infty} k^{-2n-2} B_n(t) \begin{bmatrix} \hat{a} \\ \\ \hat{b} \end{bmatrix}, \tag{5.3a}$$

$$C_n'(t),\ B_n(t) \text{ are T-periodic functions, } C_n(0) = 0 \ . \tag{5.3b}$$

The $C_n(t)$, of course, grow like $O(t)$ and provide the exponential growth of the solution; $C_n(0)$ is arbitrary since it merely scales the solution, so we pick $C_n(0) = 0$. The coefficients $P_n(t)$ in (5.2) will generally contain polynomial terms in t as a consequence of restricting the exponential part to a finite series in k^2 ; the restriction of the solution to [0,T] is therefore essential. In contrast (5.3) retains the form of an exponential multiplying a periodic function, and it should be valid over large t-regions - for instance, the periodic part should be asymptotic in k^2 to the real solution for all t.

To obtain the C_n, B_n, first define the T-periodic functions H, K, $\hat{H}$, $\hat{K}$:

$$\begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = H(t) \begin{bmatrix} a \\ b \end{bmatrix} + K(t) \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} ,$$

$$\begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} = \hat{H}(t) \begin{bmatrix} a \\ b \end{bmatrix} + \hat{K}(t) \begin{bmatrix} \hat{a} \\ \hat{b} \end{bmatrix} . \tag{5.4}$$

Substitution of (5.3a) into (1.3) gives $O(k^2)$-terms which cancel, $O(1)$-terms implying

$$C_0'(t) = H(t), \; C_0(0) = 0 \quad , \tag{5.5a}$$

$$B_0(t) = \frac{1}{2\delta} K(t) \quad ;$$

and $O(k^{-2n})$-terms, $n \geq 1$, with

$$C_n'(t) = \hat{H} \, B_{n-1}, \; C_n(0) = 0 \quad , \tag{5.5b}$$

$$B_n(t) = \frac{1}{2\delta} \left[\hat{K} \, B_{n-1} - B'_{n-1} - \sum_{m=0}^{n-1} C'_m \, B_{n-m-1} \right] .$$

All quantities in (5.5) are uniquely determined with the correct properties, so (5.3) is well-defined.

The growth rates for solutions of (1.3) should be like $\exp((-1+\delta)k^2t)$ as $k^2 \to +\infty$, and the expansion (5.3) gives the solution corresponding to the larger growth rate. If $0 < \delta < 1$, then the solution given by (5.3) decays exponentially: the limit cycle is linearly stable as a solution of (1.1), in agreement with the rough estimate at the end of the first section for nonsingular diffusion matrices. However, the expansion also includes the case $\delta = +1$, in which case the diffusion matrix is singular. This case has not been treated in the literature, so we assume $\alpha^2 + \delta_1\delta_2 = +1$ and consider this case in more detail. The growth rate of the solution corresponding to the larger Floquet multiplier is then $\exp[C_0(t)+0(\frac{1}{k^2})t]$. From (5.5a), $C_0(t) = \bar{h}t$ + (periodic function of t), where

$$\bar{h} = \frac{1}{T}\int_0^T H(t)dt \quad .$$

Therefore, if $\alpha^2 + \delta_1\delta_2 = +1$ and $\bar{h}$ is negative (positive), the limit cycle is linearly stable (unstable) as a solution of (1.1) to all sufficiently large wave numbers k^2.

In particular, consider (1.1) with $\delta_1 = \delta_2 = 0$ and $\alpha = \pm 1$. These values in (5.1) show the eigenvalue $-1+\delta$ has the eigenvectors

$$\begin{bmatrix} 1 \\ \\ 0 \end{bmatrix} \text{ if } \alpha = +1 \text{ , and } \begin{bmatrix} 0 \\ \\ 1 \end{bmatrix} \text{ if } \alpha = -1 \text{ .}$$

Consequently,

$$H(t) = F_1(t) \text{ if } \alpha = +1 \text{ , and } H(t) = G_2(t) \text{ if } \alpha = -1 \text{ .}$$

The stability implications are summarized as

Theorem 2. Define, for $F_1(t)$ and $G_2(t)$ as given in (1.3),

$$\overline{F}_1 = \frac{1}{T}\int_0^T F_1(t)dt \text{ and } \overline{G}_2 = \frac{1}{T}\int_0^T G_2(t)dt \text{ .} \tag{5.6}$$

Then (a) if $\alpha = +1$, $\delta_1 = \delta_2 = 0$ in (1.1) and $\overline{F}_1$ is negative (positive), then the limit cycle is linearly stable (unstable) as a solution of (1.1) with respect to all sufficiently large wave numbers k^2 ;

(b) if $\alpha = -1$, $\delta_1 = \delta_2 = 0$ in (1.1) and $\overline{G}_2$ is negative (postive), then the limit cycle is linearly stable (unstable) as a solution of (1.1) with respect to all sufficiently large wave numbers k^2 .

As noted in Lemma C.2, $\overline{F}_1 + \overline{G}_2 = -\mu$, the negative Floquet exponent, so at most one of $\overline{F}_1$, $\overline{G}_2$ is positive.

For example, if $\alpha = \pm 1$ and $\delta_1 = \delta_2 = 0$ in the general $\lambda - \omega$ system (2.5), we obtain (referring to (2.6) with $k^2 = 0$):

$$\overline{F}_1 = \frac{1}{T}\int_0^T R_0 S_0 \cos(\omega_0 t) \cos(\omega_0 t + \sigma_0) dt = \frac{1}{2} R_0 \lambda'(R_0) ,$$

$$\overline{G}_2 = \frac{1}{T}\int_0^T R_0 S_0 \sin(\omega_0 t) \sin(\omega_0 t + \sigma_0) dt = \frac{1}{2} R_0 \lambda'(R_0) \quad . \tag{5.7}$$

Kinetic stability of the limit cycle required $\lambda'(R_0) < 0$, so the limit cycle is linearly stable as a solution of the reaction-diffusion equations to all large wave numbers k^2 .

For the system (2.9) with $\alpha = \pm 1$ and $b = + 1$, reference to (2.12) with $k^2 = 0$ gives

$$\overline{F}_1 = \frac{1}{T}\int_0^T a(1 - 3(U(t))^2 dt , \tag{5.8a}$$

$$\overline{G}_2 = \frac{1}{T}\int_0^T a(1 - (U(t))^2) dt \quad .$$

Here $T = 2\pi$, $U(t)$ = first component of the limit cycle = $R_0(t) \cos t$, so from (2.11),

$$(U(t))^2 = \frac{(a^2 + 1)(1 + \cos 2t)}{a^2 + 1 + a^2 \cos 2t + a \sin 2t} \quad ,$$

and $\int_0^{2\pi} (U(t))^2 dt = 2\pi$, independent of a!

Therefore,

$$\overline{F}_1 = -2a \tag{5.8b}$$

$$\overline{G}_2 = 0 \quad .$$

For $\alpha = +1$, Theorem 2 shows the limit cycle is linearly stable as a solution of (2.9), but for $\alpha = -1$, the exponential growth is given by

$$\exp[C_0(t) + \frac{1}{k^2} C_1(t) + O(\frac{1}{k^4})] \quad ,$$

where $C_0(t)$ is periodic; the limit cycle is linearly stable (unstable) if the mean value of $C_1'(t)$ is negative (positive). Using (5.5b), $C_1'(t) = \hat{H}(t)B_0(t)$ and $\hat{H}(t) = G_1(t)$, $B_0(t) = \frac{1}{2} F_2(t)$.

Using (2.12) (with $k^2 = 0$) for F_2, G_1 gives

$$\text{mean value of} \qquad C_1'(t) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} (-1 + 2a\, U(t)V(t)dt \tag{5.9}$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \left[-\frac{1}{2} + \frac{a(a^2+1) \sin 2t}{(a^2+1) + a^2 \cos 2t + a \sin 2t} \right] dt$$

$$= +\frac{1}{2} - (a^2+1)^{1/2} \quad .$$

This quantity is always negative and the limit cycle is linearly stable as a solution of (2.9) with $\alpha = -1$.

CHAPTER III

AN ANALYTIC CONSTRUCTION FOR WINFREE'S ISOCHRONS

Introduction

Let $\underset{\sim}{U}(t)$ be an orbitally stable limit cycle solution for an autonomous system of differential equations ($\underset{\sim}{u}$ is an N-vector)

$$\underset{\sim}{u}' = \underset{\sim}{F}(\underset{\sim}{u}), \tag{1.1}$$

and let $\underset{\sim}{U}(0)$ be given so the limit cycle is uniquely specified. An initial point close to the limit cycle yields a trajectory $\sim \underset{\sim}{U}(t + \phi)$ as $t \rightarrow +\infty$ where $0 \leq \phi < T$ = period of the limit cycle. The constant ϕ is called the asymptotic phase of the initial point and the surface of all points with the same asymptotic phase ϕ (which intersects the limit cycle at the point $\underset{\sim}{U}(\phi)$) has been called an isochron by A. Winfree (1974).

If a physical system possesses a stable limit cycle, then isochrons provide an especially simple way of experimentally describing the state space. The asmptotic phase of a point in the state space is a single number defined by the longtime behavior of the system, which settles into the limit cycle oscillation. Measuring the asymptotic phase of various points gives a picture of the isochron structure. Winfree (1974) develops the idea of isochrons from the point of view of the experimentalist and discusses certain experiments on glycolysis and mitosis in terms of isochrons.

Asymptotic phase is a well-known concept in the theory of ordinary differential equations. Coddington and Levinson (1955, Chapter 14) set $\underset{\sim}{u} = \underset{\sim}{U}(t) + \underset{\sim}{z}$, so that (1.1) can be rewritten as

$$\underset{\sim}{z}' = \underset{\sim}{F}'(\underset{\sim}{U}(t))\underset{\sim}{z} + \underset{\sim}{f}(t,\underset{\sim}{z}), \tag{1.2}$$

where $|\underset{\sim}{f}(t,\underset{\sim}{z})| = O(|\underset{\sim}{z}|^2)$ uniformly in t for small $|\underset{\sim}{z}|$ and smooth $\underset{\sim}{F}$. The linear part of (1.2) is the variational equation of (1.1) about the limit cycle $\underset{\sim}{U}(t)$:

$$\underset{\sim}{z}' = \underset{\sim}{F}'(\underset{\sim}{U}(t))\underset{\sim}{z}, \tag{1.3}$$

a Floquet system with $\underset{\sim}{U}'(t)$ as a periodic solution (so 0 always occurs at least once as a characteristic exponent). In Theorem 2.2 of Chapter 14, Coddington and Levinson have shown that if $N-1$ characteristic exponents of (1.3) have negative real part, then through each point $\underset{\sim}{U}(\phi)$ of the limit cycle there is an $(N-1)$-dimensional surface S (an analytic surface if $\underset{\sim}{F}(\underset{\sim}{u})$ is analytic) such that each trajectory with initial point on S is asymptotic to $\underset{\sim}{U}(t+\phi)$ as $t \to +\infty$. (That is, S is an isochron with asymptotic phase ϕ.) The proof uses the fundamental matrix of (1.3) to rewrite (1.2) as an integral equation on $(t, +\infty)$. Without loss of generality, ϕ is taken to be 0, and it is shown that -- for initial conditions $\underset{\sim}{u}(0) = \underset{\sim}{U}(0) + \underset{\sim}{z}(0)$, $|\underset{\sim}{z}(0)|$ small -- only exponentially decaying solutions $\underset{\sim}{z}(t)$ occur for (1.2) (that is, $\underset{\sim}{u}(t) \sim \underset{\sim}{U}(t)$) if $\underset{\sim}{z}(0)$ satisfies a certain condition (the equation for a surface S).

Guckenheimer (1974) listed several results on isochrons related to questions raised by Winfree (1974). Fenichel (1974, 1977) gave general results on existence and smoothness of asymptotic phase (as a function of the initial point) for invariant manifolds.

These results are existence theorems with constructive proofs, but the constructions (integral equations on $(t, +\infty)$ or Poincaré maps, for example) are quite awkward for actual computation. Winfree (1978) suggested that further work on the calculation of isochrons would be of interest, which is the motivation for this chapter.

A series expansion for solutions of (1.1) close to the limit cycle will be constructed. This expansion is the analogue for a stable limit cycle of Liapunov's expansion for solutions near a stable critical point and it yields a series expansion for the isochrons.

Liapunov proved that, if $\underset{\sim}{u}_0$ is a critical point of (1.1) such that all characteristic exponents of the linearized system at $\underset{\sim}{u}_0$ have negative real part (with other minor conditions), the solutions of (1.1) could be expressed as convergent series in the exponentially-decaying solutions of the linearized system. Lefschetz (1977, Chapter 5) presents this theorem in a slightly more general form, using systems $(\underset{\sim}{u}_0 = 0)$

$$\underset{\sim}{u}' = A\underset{\sim}{u} + \underset{\sim}{g}(t,\underset{\sim}{u}), \text{ A constant matrix, } |\underset{\sim}{g}(t,\underset{\sim}{u})| = O(|\underset{\sim}{u}|^2)$$
$$\text{uniformly in } t. \qquad (1.4)$$

Here $\underset{\sim}{g}(t,\underset{\sim}{u})$ is assumed to have a series expansion about $\underset{\sim}{u} = 0$ whose coefficients are functions of t with the series uniformly convergent on $t \geq 0$. The characteristic exponents for $\underset{\sim}{z}' = A\underset{\sim}{z}$ are assumed to have negative real parts.

Lefschetz shows the solutions of (1.4) can be expressed as a convergent series in the exponentially-decaying solutions of the linearized system. Because (1.4) is nonautonomous, the coefficients in the series become indefinite integrals over $(t, +\infty)$ of quantities involving the coefficients of the expansion of $\underset{\sim}{g}(t,\underset{\sim}{u})$.

The expansion here is based on that of Lefschetz for (1.4). Two new points arise, however. First, the presence of a periodic solution in (1.2) implies that the matrix A in (1.4) has a 0-eigenvalue (and the remaining N-1 eigenvalues are taken to have negative real parts). Second, because of the underlying periodicity in the problem the t-dependent coefficients can be simplified to T-periodic functions expressed as indefinite integrals over $[0,T]$.

The main emphasis of this chapter is on two-component systems because the variational equation (1.3) is relatively easy to solve (Lemma C in Appendix I). The full solution of an N-component Floquet system can be difficult to compute numerically because the exponential behavior of the solutions can cause ill-conditioning problems. If $N = 2$ and the (easily computed) limit cycle $U(t)$ is taken as known, then one solution of the Floquet system is $U'(t)$ and finding the second reduces to solving a first-order system, which is no problem. This procedure has been summed up in Lemma B.

The second section gives the series expansion for the solutions of (1.1) near the limit cycle in a 2-component system. (Convergence follows from the results of Appendix II.) The series is a power series of exponential functions with coefficients which are periodic functions of t. The expansion for the isochrons is an immediate result of this series. The third section is concerned with the computation of the periodic coefficients. A numerical procedure is given that requires minimal use of memory while yielding high accuracy in the computation of these functions. The procedure uses extrapolation formulas for integration (and it is essential here that all functions involved be periodic).

The fourth section describes computation of isochrons (using the first four terms of the series expansion) and numerical checks on them. Briefly, if the limit cycle is fairly smooth, the first four terms of the expansion give a good approximation to the isochron in a neighborhood of the limit cycle, as expected. If the limit cycle begins to develop discontinuities, however, the region of validity appears to drastically shrink in the neighborhood of the discontinuity.

Appendix II gives the formal construction and proof of convergence for N-component systems. It begins by introducing some notation for multiple power series, then makes the formal construction, obtains an iterative bound on the terms, and uses Liapunov's Lemma to show the iterative bound leads to a majorant series for the expansion, thus proving convergence.

Expansion for the Two-Component System

The two-component case of (1.1) will be written as

$$u' = F(u,v),$$
$$v' = G(u,v), \tag{2.1}$$

with limit cycle $(U(t), V(t))$ of period T and $(U(0), V(0))$ specified. The variational equation of (2.1) about the limit cycle is the Floquet system

$$\begin{bmatrix} w' \\ z' \end{bmatrix} = \begin{bmatrix} F_u(U(t), V(t)) & F_v(U(t), V(t)) \\ G_u(U(t), V(t)) & G_v(U(t), V(t)) \end{bmatrix} \begin{bmatrix} w \\ z \end{bmatrix}, \tag{2.2}$$

with fundamental matrix given by Lemma C:

$$\begin{bmatrix} U'(t) & \hat{U}(t)\exp(-\mu t) \\ V'(t) & \hat{V}(t)\exp(-\mu t) \end{bmatrix}, \quad U', V', \hat{U}, \hat{V} \text{ T-periodic functions.} \tag{2.3}$$

A series expansion

$$\begin{bmatrix} u \\ v \end{bmatrix} = \sum_{n=0}^{\infty} \epsilon^n \begin{bmatrix} u_n \\ v_n \end{bmatrix} \tag{2.4}$$

is assumed for u,v and is substituted into (2.1). Our choice below of (u_0,v_0) as the limit cycle gives ϵ the interpretation of a measure of the derivation of the solution from the limit cycle. Notice that the formal result of such a substitution yields (with similar results for $G(u,v)$):

$$F(u,v) = F(u_o,v_o) + (F_u(u_o,v_o)u_1 + F_v(u_o,v_o)v_1)\epsilon$$

$$+ \sum_{n=2}^{\infty} \Big[F_u(u_o,v_o)\, u_n + F_v(u_o,v_o)v_n$$

$$+ F_n\,(u_o, \ldots, u_{n-1}, v_o, \ldots, v_{n-1})\Big]\,\epsilon^n \qquad (2.5a)$$

$F_n(u_o, \ldots, u_{n-1}, v_o, \ldots, v_{n-1})$ is a polynomial in the variables $u_1, \ldots, u_{n-1}, v_1, \ldots, v_{n-1}$ and satisfies the <u>homogeneity property</u>,

$$F_n(u_o, ku_1, k^2u_2, \ldots, k^{n-1}u_{n-1}, v_o, kv_1, \ldots, k^{n-1}v_{n-1})$$

$$= k^n\, F_n(u_o, u_1, \ldots, u_{n-1}, v_o, \ldots, v_{n-1}). \qquad (2.5b)$$

(It is assumed that F, G are analytic -- it is sufficient that they be analytic at each point of the limit cycle.)

Substitution of (2.4) into (2.1) and applying the notation of (2.5a) give

$$\begin{bmatrix} u_o' \\ v_o' \end{bmatrix} = \begin{bmatrix} F(u_o,v_o) \\ G(u_o,v_o) \end{bmatrix} \text{ with solution } \begin{bmatrix} u_o \\ v_o \end{bmatrix} = \begin{bmatrix} U(t+\phi) \\ V(t+\phi) \end{bmatrix}, \qquad (2.6a)$$

$$\begin{bmatrix} u_1' \\ v_1' \end{bmatrix} = \begin{bmatrix} F_u(U(t+\phi),\ V(t+\phi)) & F_v(U(t+\phi),\ V(t+\phi)) \\ G_u(U(t+\phi),\ V(t+\phi)) & G_v(U(t+\phi),\ V(t+\phi)) \end{bmatrix} \begin{bmatrix} u_1 \\ v_1 \end{bmatrix},$$

(2.6b)

$$\begin{bmatrix} u_n' \\ v_n' \end{bmatrix} = \begin{bmatrix} F_u(U(t+\phi),\ V(t+\phi)) & F_v(U(t+\phi),\ V(t+\phi)) \\ G_u(U(t+\phi),\ V(t+\phi)) & G_v(U(t+\phi),\ V(t+\phi)) \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix}$$

$$+ \begin{bmatrix} F_n(u_o,\ \ldots,\ u_{n-1},\ v_o,\ \ldots,\ v_{n-1}) \\ G_u(u_o,\ \ldots,\ u_{n-1},\ v_o,\ \ldots,\ v_{n-1}) \end{bmatrix}. \tag{2.6c}$$

The idea of the substitution is to pick u_o, v_o as the limit cycle (as above) and then require all subsequent u_n, v_n to decay exponentially. Obviously we should choose

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \exp(-\mu(t+\phi)) \begin{bmatrix} U(t+\phi) \\ V(t+\phi) \end{bmatrix}. \tag{2.7}$$

(It will be notationally convenient to write solutions as functions of $t+\phi$; the factor $\exp(-\mu\phi)$ will eventually be absorbed into ϵ.)

We now show that all terms u_n, v_n in the expansion can be written in the form

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = \exp(-n\mu(t+\phi)) \begin{bmatrix} U_n(t+\phi) \\ V_n(t+\phi) \end{bmatrix},$$

U_n, V_n T-periodic functions. (2.8)

The argument is by induction; notice (2.8) already holds for $n = 0, 1$.

Given $n \geq 2$, assuming (2.8) holds for u_m, v_m with $m < n$, and using the homegenity property of F_n, G_n in (2.5b), (2.6c) becomes:

$$\begin{bmatrix} u_n' \\ v_n' \end{bmatrix} = \begin{bmatrix} F_u(U(t+\phi), V(t+\phi)) & F_v(U(t+\phi), V(t+\phi)) \\ G_u(U(t+\phi), V(t+\phi)) & G_v(U(t+\phi), V(t+\phi)) \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix}$$

$$+ \exp(-n\ (t+\phi)) \begin{bmatrix} F_n(U_o(t+\phi), \ldots, U_{n-1}(t+\phi), \\ G_n(U_o(t+\phi), \ldots, U_{n-1}(t+\phi), \end{bmatrix}$$

$$\begin{matrix} V_o(t+\phi), \ldots, V_{n-1}(t+\phi)) \\ V_o(t+\phi), \ldots, V_{n-1}(t+\phi)) \end{matrix}\Bigg] . \qquad (2.9)$$

Referring to Lemma D for the solution of (2.9), we are led to define two T-periodic function $\hat{F}_n(t)$, $\hat{G}_n(t)$ by:

$$\begin{bmatrix} c_n + \exp(-n\mu t)\ \hat{F}_n(t) \\ d_n + \exp(-(n-1)\mu t)\hat{G}_n(t) \end{bmatrix} = \int_0^t \begin{bmatrix} \hat{V}(s) & -\hat{U}(s) \\ -\exp(\mu s)V'(s) & \exp(\mu s)U'(s) \end{bmatrix}$$

$$\begin{bmatrix} F_n(U_o(s), \ldots, U_{n-1}(s), \ldots, V_{n-1}(s)) \\ G_n(U_o(s), \ldots, U_{n-1}(s), \ldots, V_{n-1}(s)) \end{bmatrix}$$

$$\frac{\exp(-n\mu s)\ ds}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)}, \quad n \geq 2. \qquad (2.10)$$

(The form of the expression on the left follows from Lemma A.) Then the solution of (2.9) can be written as

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = \begin{bmatrix} U'(t+\phi)\ \exp\,(-\mu(t+\phi))U(t+\phi) \\ V'(t+\phi)\ \exp\,(-\mu(t+\phi))V(t+\phi) \end{bmatrix}$$

$$\cdot \begin{bmatrix} \exp\,(-n\mu(t+\phi))\ \hat{F}_n\,(t+\phi) \\ \exp(-(n-1)\mu(t+\phi))\ \hat{G}_n\,(t+\phi) \end{bmatrix}$$

$$= \exp\,(-n\mu(t+\phi)) \begin{bmatrix} U_n(t+\phi) \\ V_n(t+\phi) \end{bmatrix}, \qquad (2.11)$$

as claimed.

If we combine $\epsilon \exp(-\mu\phi)$ together as a single quantity ϵ, the results can be summarized as

THEOREM 1. The solution of (2.1) can be written formally as

$$\begin{bmatrix} u \\ v \end{bmatrix} = \sum_{n=0}^{\infty} \epsilon^n \exp\,(-n\mu t) \begin{bmatrix} U_n(t+\phi) \\ V_n(t+\phi) \end{bmatrix}, \qquad (2.12a)$$

where $U_n(t)$, $V_n(t)$ are T-periodic functions given by

$$(U_o(t), V_o(t)) = (U(t), V(t)) \quad \text{(the limit cycle);} \qquad (2.12b)$$

$$(U_1(t), V_1(t)) = (\hat{U}(t), \hat{V}(t)) \quad \text{(given by Lemma C, which also gives } \mu\text{);} \qquad (2.12c)$$

$$\begin{bmatrix} U_n(t) \\ V_n(t) \end{bmatrix} = \hat{F}_n(t) \begin{bmatrix} U'(t) \\ V'(t) \end{bmatrix} + \hat{G}_n(t) \begin{bmatrix} \hat{U}(t) \\ \hat{V}(t) \end{bmatrix}$$

$$(\hat{F}_n,\ \hat{G}_n \text{ given by (2.10), } n \geq 2). \tag{2.12d}$$

(NOTE: convergence of the expansion for small $|\epsilon|$ is proven in Appendix II).

Notice that a solution given by (2.12) is asymptotic to $U(t + \phi)$, $V(t + \phi)$ with asymptotic phase ϕ, so the initial points lie on the isochron corresponding to ϕ. The initial points are found by setting $t = 0$, giving

COROLLARY 1. The isochron corresponding to asymptotic phase ϕ is the curve $(u(\epsilon), v(\epsilon))$ given by

$$\begin{bmatrix} u(\epsilon) \\ v(\epsilon) \end{bmatrix} = \sum_{n=0}^{\infty} \epsilon^n \begin{bmatrix} U_n(\phi) \\ V_n(\phi) \end{bmatrix}. \tag{2.13}$$

It is instructive to compare these expansions (2.12) and (2.13) for the trajectories and isochrons with explicit solutions. The system ($R^2 = u^2 + v^2$)

$$\begin{bmatrix} u' \\ v' \end{bmatrix} = \begin{bmatrix} 1 - R^2 & -\frac{1}{2}(1 + R^2) \\ \frac{1}{2}(1 + R^2) & 1 - R^2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \tag{2.14a}$$

transforms using $u = R\cos\psi$, $v = R\sin\psi$ to

$$R' = R(1 - R^2)$$

$$\psi' = \frac{1}{2}(1 + R^2). \tag{2.14b}$$

These two equations can be integrated exactly, introducing 2 constants of integration, written as ϵ, ϕ in the following results for the trajectories:

$$R = [1 + 2\,\epsilon\,\exp(-2t)]^{-1/2}$$

$$\psi = (t + \phi) + \frac{1}{4}\,\ell n\,|1 + 2\,\epsilon\,\exp(-2t)| \tag{2.14c}$$

Expanding as a series in powers of $\epsilon\,\exp(-2t)$ yields a series like that of Theorem 1:

$$\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \cos(t + \phi) \\ \sin(t + \phi) \end{bmatrix} + \exp(-2t)\begin{bmatrix} -\cos(t + \phi) - \frac{1}{2}\sin(t + \phi) \\ \frac{1}{2}\cos(t + \phi) - \sin(t + \phi) \end{bmatrix}$$
$$+ \epsilon^2 \exp(-4t)\begin{bmatrix} \frac{11}{8}\cos(t + \phi) + \sin(t + \phi) \\ -\cos(t + \phi) + \frac{11}{8}\sin(t + \phi) \end{bmatrix}$$
$$+ \epsilon^3 \exp(-6t)\begin{bmatrix} -\frac{17}{8}\cos(t + \phi) - \frac{91}{48}\sin(t + \phi) \\ +\frac{91}{48}\cos(t + \phi) - \frac{17}{8}\sin(t + \phi) \end{bmatrix}$$
$$+ O(\epsilon^4 \exp(-8t)). \tag{2.14d}$$

The *isochron* for asymptotic phase ϕ is given exactly by

$$\begin{bmatrix} u(\epsilon) \\ v(\epsilon) \end{bmatrix} = \begin{bmatrix} (1 + 2\epsilon)^{-1/2} \cos(\phi + \frac{1}{4} \ln|1 + 2\epsilon|) \\ (1 + 2\epsilon)^{-1/2} \sin(\phi + \frac{1}{4} \ln|1 + 2\epsilon|) \end{bmatrix}, \tag{2.14e}$$

with a series expansion given by setting $t = 0$ in (2.14d).

This example and the van der Pol oscillator will be used as test cases for the numerical work in the next few sections. The question to be considered next is an efficient way of calculating the periodic coefficients $U_n(t)$, $V_n(t)$.

The Numerical Method for the Periodic Coefficients

The calculation of the T-periodic coefficients $U_n(t)$, $V_n(t)$ in (2.12) or (2.13) requires the calculation of the T-periodic functions $\hat{F}_n(t)$, $\hat{G}_n(t)$ in (2.10). Basically, the problem is a recursion of the form

$f_0(t)$ is a given T-periodic function;

$$f_n(t) = \exp(+n\mu t)\left[\int_0^t \exp(-n\mu s)\, A_n(f_0(s), f_1(s), \ldots, f_{n-1}(s))ds - c_n\right],$$

with c_n such that $f_n(t)$ is T-periodic. (3.1)

Here $f_0(t)$ corresponds to the limit cycle $(U(t), V(t))$, i.e., (U_0, V_0); the calculation of $f_1(t)$ corresponds to the calculation required in Lemma C.5, determining $(\hat{U}, \hat{V})$, i.e., (U_1, V_1); and the calculation of $f_n(t)$ corresponds to the recursion in (2.10). Certain points have already been made following Lemma A in Appendix I about the evaluation of integrals of the form (3.1), for instance, that c_n is easily calculated (Lemma A.2b) and that if $\mu > 0$ (as it is here) backwards integration in t is helpful to avoid ill-conditioning problems, as described in (App. I.3). The discussion in Appendix I refers to the evaluation of a single integral of the form (3.1). Here the problem involves a sequence of such evaluations and the necessity of retaining all the functions f_0, f_1, f_2, ... raises a storage problem (if high accuracy is sought).

Suppose we wish to calculate f_0, f_1, f_2, f_3 so that $f_3(t)$ is tabulated at N points over the interval $[0,T]$, that is, at steps of length $h = T/N$. Using (App. I.3) to evaluate the integral in (3.1), we still have to choose a means of evaulating an integral over one step $[(n-1)h, nh]$. Consider the following rules (Birkhoff and Rota, 1969, Chapter 7)

$$\int_a^{a+h} p(t)\, dt = \frac{h}{2}\,[p(a) + p(a+h)] + O(h^3) \tag{3.2a}$$

$$= \frac{h}{6} \; [p(a) + 4\, p(a + \frac{h}{2}) + p(a + h)] + O(h^5) \qquad (3.2b)$$

$$= \frac{h}{8} \; [p(a) + 3\, p(a + \frac{h}{3}) + 3\, p(a + \frac{2h}{3}) + p(a + h)]$$

$$+ O(h^7) \qquad (3.2c)$$

The relative error in applying these functions over the interval $[0,T]$ will be $O(h^2)$, $O(h^4)$, $O(h^6)$ respectively.

In using (3.2a), only 4N memory locations are needed to retain the tabulated points for f_0, f_1, f_2, f_3; the errors in f_1, f_2, f_3 will be $O(h^2)$.

In using the more accurate (3.2b), however, 15N memory spaces will be necessary because f_0 must be tabulated at 8N points to give f_1 at 4N points (since midpoints disappear in the process), which gives f_2 at 2N points, which gives f_3 at N points. The error for each f_i here is $O(h^4)$.

For the still more accurate formula (3.2c), 40N memory spaces are needed to give $O(h^6)$ accuracy. In general, to obtain a relative error $O(h^{2k})$ for coefficients f_0, f_1, ..., f_m, with f_m to be tabulated at N points, requires an interpolation scheme using $(k + 1)$ points on each h-interval (so f_{m-1} must be tabulated at kN points, ..., f_0 at $k^m N$ points). That is, using interpolation formulas,

$O(h^{2k})$ accuracy for $f_1, f_2, \ldots, f_m$ and f_m to be tabulated at

$$N \text{ points requires } \frac{k^{m+1} - 1}{k - 1} N \text{ memory spaces.} \tag{3.3}$$

In short, in using normal interpolation formulas such as (3.2) in calculating a fixed number m of coefficients, the memory required increases like Nk^m, where 2k is the order of accuracy.

We now give a method of tabulating the coefficients $f_0, \ldots, f_m$ with relative error $O(h^{2k})$ which requires only $(m+1)N$ memory spaces <u>independent of k.</u>

The idea is to derive <u>extrapolation formulas</u> to express an integral over $[(n-1)h, nh]$ by points <u>outside</u> the interval. This leads to, for example

$$\int_a^{a+h} p(t)dt = \frac{h}{24} [- p(a-h) + 13\, p(a) + 13\, p(a+h) - p(a+2h)] + O(h^3) \tag{3.4}$$

with the coefficients derived in the usual way (Birkhoff and Rota, Chapter 7) by expanding in Taylor series (around $a + h/2$, for instance) and canceling powers of h. Such an exterior formula would cause trouble near endpoints, where $p(a + 2h)$ might run outside tabulated values, but since all functions here are periodic on $[0,T]$, <u>there are no endpoints.</u>

Using (3.4) to evaluate the integral in (3.1) permits the calculation of f_0, f_1, f_2, f_3 with accuracy $O(h^4)$ for each function using only 4N memory spaces instead of 15N. Similarly, such extrapolation formulas with higher orders of accuracy require no increase in memory storage, as long as the number of points used, which is 2k for $O(h^{2k})$, is small compared with N. This is no problem in practice since N will be > 100 and accuracy of $O(h^{100})$ is seldom required.

Numerical Calculations

In this section the first four terms of the isochron expansion (2.13) in Corollary 1 will be calculated numerically for two examples. The first example is

$$u' = (1 - R^2)u - \frac{1}{2}(1 + R^2)v$$

$$v' = \frac{1}{2}(1 + R^2)u + (1 - R^2)v, \tag{4.1}$$

which has already been mentioned at the end of the second section. It provides a useful check because its isochrons and the coefficients $U_n(\phi)$, $V_n(\phi)$ in (2.13) can be found explicitly from (2.14e).

The second example is the van der Pol oscillator

$$u' = \lambda u(1 - u^2/3) - v, \quad \lambda > 0$$

$$v' = u \tag{4.2}$$

which is chosen to examine the expansion for smooth limit cycles (small λ) and "discontinuous" ones (large λ). *In this case the* isochrons are checked by taking points on the approximation and finding their asymptotic phase by direct integration.

The numerical work used two Fortran programs. The first program simply found a point $u > 0$, $v = 0$ on the limit cycle (to be used as a starting point for the second program) and the limit cycle period T. It worked as follows:

1. An initial guess $(u,v) = (u_0, 0)$ with $u_0 > 0$ is made for a point on the limit cycle.
2. Runge-Kutta integration is applied until the trajectory crosses the positive u-axis. (It is assumed that the limit cycle encircles the origin.)
3. As soon as the positive u-axis is crossed, the program backs up to the point of crossing along a tangent line approximation. The result is a new starting point $(u,v) = (u_1, 0)$ with $u_1 > 0$ and an approximate period T.
4. Steps (1)-(3) are now repeated to obtain a sequence of starting points $(u,v) = (u_n, 0)$ with $u_n > 0$ and approximate periods T_n.

5. From stability of the limit cycles, we expect the points $(u_n, 0)$ to converge to a point on the limit cycle and the $T_n \to T$, so the interation stops when u_n, u_{n-1} are very close (typically, within 10^{-6}).

The second program uses the final values $(u_n, 0)$, T_n from the first program as $(U(0), V(0))$, T -- that is, a starting point and period for the limit cycle -- and then calculates $U_n(t)$, $V_n(t)$ for $n = 0, 1, 2, 3$. It proceeds as:

1. $(U(t), V(t))$, i.e., $(U_0(t), V_0(t))$, is tabulated at intervals of $h = T/N$ using a Runge-Kutta method; $(U'(t), V'(t))$ is tabulated directly from (U,V) using the kinetic system. (As shown in the third section, the use of an extrapolation formula for the integration permits all relevant functions to be tabulated at the same intervals.)
2. The Floquet exponent μ is found using Lemma C.2.
3. The coefficients $A(t)$, $B(t)$ in Lemma C.4-5 are tabulated; then $(U(t), V(t))$, i.e., $(U_1(t), V_1(t))$ is found from Lemma C.3.
4. The periodic functions $\hat{F}_2(t)$, $\hat{G}_2(t)$ are calculated from (2.10) using the results of Lemma A; these functions then give $(U_2(t), V_2(t))$ using (2.11).
5. $\hat{F}_3(t)$, $\hat{G}_3(t)$, $(U_3(t), V_3(t))$ are found as in (4).

Steps (4) and (5) required the following explicit expressions for the functions in the expansion (2.5):

$$F_2(u_0,u_1;v_0,v_1) = \frac{1}{2}\left[F_{uu}(u_0,v_0)u_1{}^2 + 2\,F_{uv}(u_0,v_0)u_1v_1 + F_{vv}(u_0,v_0)v_1{}^2\right],$$

$$\begin{aligned} F_3(u_0,u_1,u_2;\ v_0,v_1,v_2) &= F_{uu}(u_0,v_0)u_1u_2 + F_{uv}(u_0,v_0)\ (u_1v_2 + u_2v_1) \\ &+ F_{vv}(u_0,v_0)v_1v_2 + \frac{1}{6}\Big[F_{uuu}(u_0,v_0)u_1{}^3 + 3\,F_{uuv}(u_0,v_0)u_1{}^2v_1 \\ &+ 3F_{uvv}(u_o,v_o)u_1v_1^2 + F_{vvv}(u_0,v_0)v_1{}^3\Big], \end{aligned} \tag{4.3}$$

with corresponding expressions for G_2,G_3.

The results for the first example (4.1) are shown in Table 1, which compares the coefficients $U_n(t),V_n(t)$ as calculated numerically with the exact values obtained by expanding (2.14e)--the agreement is excellent. Figure 3 shows an exact isochron drawn from (2.14e) and an approximate isochron drawn using the first four terms (through $O(\epsilon^3)$) of the expansion (2.13); again, the two curves are in excellent agreement for $|\epsilon|$ small (points close to the limit cycle).

The next calculations are for the van der Pol oscillator (4.2) with $\lambda = .5,\ 1.0$. These small values of λ give fairly smooth limit cycles shown in Figure 4. The coefficients, given at intervals

TABLE 1

COMPARISON OF NUMERICAL CALCULATIONS AND EXACT VALUES FOR THE COEFFICIENT $U_n(t)$, $V_n(t)$ IN THE EXPANSION (2.12) FOR THE SYSTEM (2.14)

NUMBERICAL SOLUTIONS					EXACT VALUES				
t /T	$U_o(t)$ / $V_o(t)$	U_1 / V_1	U_2 / V_2	U_3 / V_3	t /T	$V_o(t)$ / $U_o(t)$	V_1 / U_1	V_2 / U_2	V_3 / U_3
.0	1.0000	-1.0000	1.3750	-2.1250	.0	1.0000	-1.0000	1.3750	-2.1250
	.0000	.5000	-1.0000	1.8958		.0000	.5000	-1.0000	1.8958
.1	.8090	-1.1029	1.7001	-2.8333	.1	.8090	-1.1029	1.7002	-2.8335
	.5878	-1.8328	- .0008	.2847		.5878	- .1833	- .0008	.2847
.2	.3090	- .7845	1.3759	-2.4594	.2	.3090	- .7845	1.3760	-2.4597
	.9511	- .7965	.9986	-1.4350		.9511	- .7965	.9987	-1.4352
.3	- .3090	- .1665	.5261	-1.1462	.3	- .3090	- .1665	.5262	-1.1464
	.9511	-1.1055	1.6166	-2.6064		.9511	-1.1056	1.6167	-2.6068
.4	- .8090	.5151	- .5245	.0647	.4	- .8090	.5151	- .5262	.6048
	.5878	- .9922	1.6170	-2.7823		.5878	- .9923	1.6172	-2.7828
.5	-1.0000	.9999	-1.3748	2.1245	.5	-1.0000	1.0000	-1.3750	2.1250
	.0000	- .5000	.9998	-1.8954		.0000	- .5000	1.0000	-1.8958
.6	- .8090	1.1028	-1.6999	2.8327	.6	- .8090	1.1029	-1.7002	2.8335
	- .5878	0.1833	.0008	- .2846		- .5878	.1833	.0008	- .2847
.7	- .3090	.7845	-1.3757	2.4589	.7	- .3090	.7845	-1.3760	2.4597
	- .9511	.7965	- .9985	1.4347		- .9511	.7954	- .9987	1.4352
.8	.3090	.1665	- .5260	1.1460	.8	.3090	.1665	- .5262	1.1464
	- .9511	1.1054	-1.6163	2.6059		- .9511	1.1056	-1.6167	2.6068
.9	.8090	- .5151	.5245	- .6046	.9	.8090	- .5151	.5246	- .6048
	- .5878	.9922	-1.6168	2.7818		- .5878	.9923	-1.6172	2.7828
1.0	1.0000	- .9999	1.3747	-2.1246	1.0	1.0000	-1.0000	1.3750	-2.1250
	- .0000	.4999	- .9999	1.8956		.0000	.5000	-1.0000	1.8958

$$u = (1-R^2)u \quad - \frac{1}{2}(1+R^2)v$$

$$v = \frac{1}{2}(1+R^2)u + \quad (1-R^2)v$$

period T = 2 Floquet exponent = 2

step size = T/200

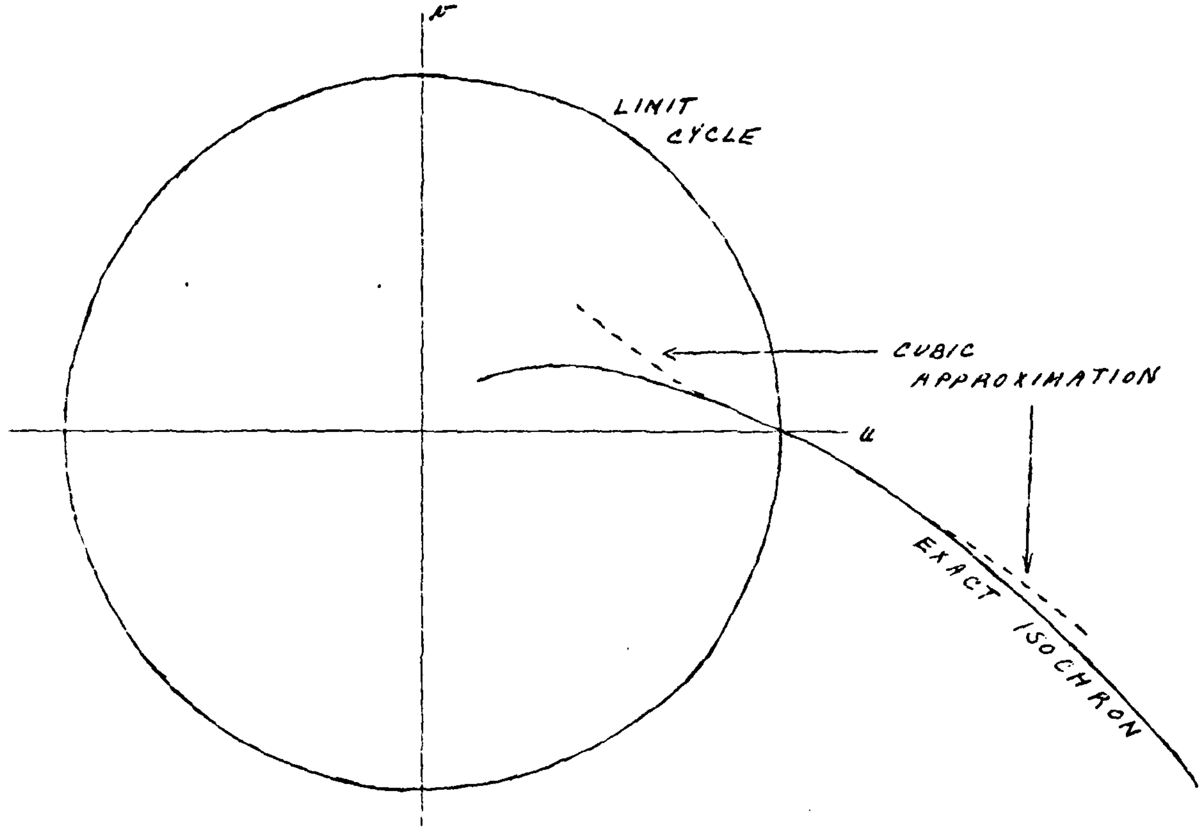


FIGURE 3. COMPARISON OF AN EXACT ISOCHRON WITH THE NUMERICALLY CALCULATED APPROXIMATION (BASED ON TERMS THROUGH $\mathcal{O}(\epsilon^3)$) FOR THE SYSTEM $\dot{R} = \mu(1-R^2)$, $\dot{\psi} = \frac{1}{2}(1+R^2)$. (TO SCALE.)

of .1T, for the first four terms of the isochron expansion (2.13) are given in Tables 2A, 2B. Using the coefficients, the cubic approximation

$$\begin{bmatrix} u(\epsilon) \\ v(\epsilon) \end{bmatrix} = \sum_{n=0}^{3} \begin{bmatrix} U_n(\phi) \\ V_n(\phi) \end{bmatrix} \epsilon^n$$

is found; these approximate isochrons have been sketched for the values $\phi = 0$, .3T in Figure 4.

As a check of these isochrons, points on the approximate curves $u(\epsilon), v(\epsilon)$ for $\lambda = .5$, 1.0 and $\phi = 0$, .3T were chosen by picking various values of ϵ. These points were integrated to $t = +\infty$ (in practice, to t = 5T) where they were practically on the limit cycle, thereby determining their asymptotic phase for the approximate points $u(\epsilon), v(\epsilon)$ and the intended asymptotic phase (either 0 or .3T) is found and given in Table 3--the difference should be close to 0 and it is. (The "absolute distance" in Table 3 is the distance between the computed point at t = 5T and the ideal point at (U(0),V(0)) or (U(.3T),V(.3T)); dividing this (small) distance by $((u')^2 + (v')^2)^{1/2}$ gives the phase difference.)

For larger values of λ the limit cycle in (4.2) begins to develop corners and one expects something curious to happen in the expansion. Tables 2C, 2D give the coefficients for $\lambda = 2,4$; notice the enormous size of the coefficients for $\phi = .3T$ and .8T (points near the

TABLE 2

THE COEFFICIENTS $U_n(t)$, $V_n(t)$, $n = 0, 1, 2, 3$, IN THE EXPANSION (2.12) FOR VARIOUS VALUES OF THE PARAMETER IN THE VAN DER POL EQUATION

$$u = -v + \lambda u\left(1 - \frac{u^2}{3}\right)$$

$$v = u$$

TIME/T	U0 / V0	U1 / V1	U2 / V2	U3 / V3
0.0	0.19762E+01	-0.50780E+00	0.20129E+00	-0.89280E-01
	0.0	0.11687E-01	-0.13274E-01	0.75555E-02
0.1	0.15437E+01	-0.26998E+00	0.76494E-01	-0.24351E-01
	0.11458E+01	-0.26305E+00	0.91137E-01	-0.36292E-01
0.2	0.72995E+00	-0.57201E-01	-0.14687E-01	0.22414E-01
	0.18915E+01	-0.48756E+00	0.20725E+00	-0.10383E+00
0.3	-0.50794E+00	0.39066E+00	-0.30636E+00	0.25065E+00
	0.19847E+01	-0.57921E+00	0.28998E+00	-0.17418E+00
0.4	-0.17322E+01	0.75178E+00	-0.48406E+00	0.34581E+00
	0.12358E+01	-0.35648E+00	0.16791E+00	-0.89995E-01
0.5	-0.19762E+01	0.50752E+00	-0.20176E+00	0.90092E-01
	0.10967E-03	-0.99720E-02	0.12079E-01	-0.68069E-02
0.6	-0.15438E+01	0.26996E+00	-0.76488E-01	0.24350E-01
	-0.11457E+01	0.26303E+00	-0.91130E-01	0.36289E-01
0.7	-0.73003E+00	0.57201E-01	0.14686E-01	-0.22409E-01
	-0.18914E+01	0.48752E+00	-0.20723E+00	0.10383E+00
0.8	0.50781E+00	-0.39062E+00	0.30633E+00	-0.25063E+00
	-0.19847E+01	0.57916E+00	-0.28996E+00	0.17417E+00
0.9	0.17321E+01	-0.75175E+00	0.48408E+00	-0.34586E+00
	-0.12359E+01	0.35644E+00	-0.16786E+00	0.89974E-01
1.0	0.19762E+01	-0.50776E+00	0.20126E+00	-0.89274E-01
	-0.21875E-03	0.11712E-01	-0.13281E-01	0.75589E-02

Table 2A	Parameter =	0.50000 = λ
	Period =	6.38057 = T
	Floquet Exponent =	0.50768 = μ
	Step Size = Period/	200

TABLE 2 (Continued)

THE COEFFICIENTS $U_n(t)$, $V_n(t)$, $n = 0, 1, 2, 3$, IN THE EXPANSION (2.12) FOR VARIOUS VALUES OF THE PARAMETER IN THE VAN DER POL EQUATION

$$\dot{u} = -v + \lambda u \left(1 - \frac{u^2}{3}\right)$$

$$\dot{v} = u$$

TIME/T	U0 V0	U1 V1	U2 V2	U3 V3
0.0	0.19193E+01 0.0	-0.52851E+00 0.32829E-01	0.23850E+00 -0.25402E-01	-0.12049E+00 0.12788E-01
0.1	0.15050E+01 0.11532E+01	-0.22479E+00 -0.24555E+00	0.69028E-01 0.89357E-01	-0.25312E-01 -0.39361E-01
0.2	0.83313E+00 0.19512E+01	-0.48770E-02 -0.59608E+00	-0.70484E-01 0.39381E+00	0.94490E-01 -0.32756E+00
0.3	-0.41537E+00 0.21370E+01	0.10781E+01 -0.88997E+00	-0.18418E+01 0.94868E+00	0.34467E+01 -0.13525E+01
0.4	-0.18707E+01 0.13137E+01	0.15550E+01 -0.47182E+00	-0.18960E+01 0.32350E+00	0.25429E+01 -0.28634E+00
0.5	-0.19193E+01 0.69678E-04	0.52863E+00 -0.33509E-01	-0.24073E+00 0.24558E-01	0.12415E+00 -0.11833E-01
0.6	-0.15050E+01 -0.11531E+01	0.22477E+00 0.24551E+00	-0.69019E-01 -0.89332E-01	0.25308E-01 0.39345E-01
0.7	-0.83318E+00 -0.19511E+01	0.49026E-02 0.59598E+00	0.70447E-01 -0.39371E+00	-0.94437E-01 0.32743E+00
0.8	0.41528E+00 -0.21370E+01	-0.10778E+01 0.88988E+00	0.18412E+01 -0.94851E+00	-0.34452E+01 0.13521E+01
0.9	0.18707E+01 -0.13138E+01	-0.15549E+01 0.47181E+00	0.18960E+01 -0.32350E+00	-0.25430E+01 0.28637E+00
1.0	0.19193E+01 -0.13685E-03	-0.52845E+00 0.32849E-01	0.23844E+00 -0.25409E-01	-0.12048E+00 0.12792E-01

Table 2B

Parameter = 1.00000 = λ

Period = 6.66321 = T

Floquet Exponent = 1.05931 = μ

Step Size = Period/ 200

TABLE 2 (Continued)

THE COEFFICIENTS $U_n(t)$, $V_n(t)$, n = 0, 1, 2, 3, IN THE EXPANSION (2.12) FOR VARIOUS VALUES OF THE PARAMETER IN THE VAN DER POL EQUATION

$$\dot{u} = -v + \lambda u\left(1 - \frac{u^2}{3}\right)$$

$$\dot{v} = u$$

TIME/T	U0 V0	U1 V1	U2 V2	U3 V3
0.0	0.18171E+01 0.0	-0.56831E+00 0.89378E-01	0.30829E+00 -0.35797E-01	-0.18306E+00 0.15225E-01
0.1	0.14927E+01 0.12691E+01	-0.21745E+00 -0.17074E+00	0.11268E+00 0.65832E-01	-0.65164E-01 -0.32648E-01
0.2	0.99168E+00 0.22354E+01	0.77857E-01 -0.11644E+01	-0.20069E+00 0.28448E+01	0.95404E+00 -0.86358E+01
0.3	-0.33267E+00 0.25967E+01	0.11730E+02 -0.36895E+01	-0.18713E+03 0.51369E+02	0.36096E+04 -0.85019E+03
0.4	-0.20197E+01 0.14787E+01	0.54060E+01 -0.10625E+01	-0.20738E+02 0.19792E+01	0.88074E+02 -0.54636E+01
0.5	-0.18172E+01 0.13256E-03	0.56951E+00 -0.95624E-01	-0.31650E+00 0.37060E-01	0.19840E+00 -0.14981E-01
0.6	-0.14927E+01 -0.12689E+01	0.21741E+00 0.17066E+00	-0.11261E+00 -0.65770E-01	0.65103E-01 0.32603E-01
0.7	-0.99174E+00 -0.22354E+01	-0.77739E-01 0.11639E+01	0.20031E+00 -0.28424E+01	-0.95217E+00 0.86246E+01
0.8	0.33244E+00 -0.25967E+01	-0.11722E+02 0.36887E+01	0.18694E+03 -0.51338E+02	-0.36046E+04 0.84934E+03
0.9	0.20197E+01 -0.14789E+01	-0.54059E+01 0.10627E+01	0.20739E+02 -0.19794E+01	-0.88088E+02 0.54646E+01
1.0	0.18172E+01 -0.26613E-03	-0.56819E+00 0.89407E-01	0.30818E+00 -0.35807E-01	-0.18302E+00 0.15234E-01

Table 2C	Parameter =	2.00000 = λ
	Period =	7.62973 = T
	Floquet Exponent =	2.38245 = μ
	Step Size = Period/	200

TABLE 2 (Continued)

THE COEFFICIENTS $U_n(t)$, $V_n(t)$, $n = 0, 1, 2, 3$, IN THE EXPANSION (2.12) FOR VARIOUS VALUES OF THE PARAMETER IN THE VAN DER POL EQUATION

$$u = -v + \lambda u \left(1 - \frac{u^2}{3}\right)$$

$$v = u$$

TIME/T	U0 V0	U1 V1	U2 V2	U3 V3
0.0	0.17572E+01	-0.57722E+00	0.29671E+00	-0.16810E+00
	0.0	0.69474E-01	-0.18288E-01	0.69732E-02
0.1	0.15186E+01	-0.19318E+00	0.65358E-01	-0.22850E-01
	0.16768E+01	0.26823E-02	-0.34531E-02	0.10564E-02
0.2	0.11566E+01	-0.28349E+00	0.32962E+02	-0.83993E+03
	0.30598E+01	-0.50499E+01	0.11999E+03	-0.32753E+04
0.3	-0.52209E+00	0.54159E+04	-0.35752E+08	0.28486E+12
	0.37352E+01	-0.21692E+03	0.34843E+07	-0.26968E+11
0.4	-0.19481E+01	0.36367E+02	-0.94882E+03	0.27602E+05
	0.18934E+01	-0.46555E+01	0.61528E+02	-0.12112E+04
0.5	-0.17572E+01	0.57707E+00	-0.30418E+00	0.18354E+00
	0.20627E-03	-0.73095E-01	0.19259E-01	-0.72312E-02
0.6	-0.15186E+01	0.19292E+00	-0.65168E-01	0.22749E-01
	-0.16766E+01	-0.26903E-02	0.34441E-02	-0.10517E-02
0.7	-0.11566E+01	0.28352E+00	-0.32850E+02	0.83549E+03
	-0.30597E+01	0.50401E+01	-0.11952E+03	0.32561E+04
0.8	0.52144E+00	-0.54030E+04	0.35603E+08	-0.28319E+12
	-0.37353E+01	0.21716E+03	-0.34752E+07	0.26836E+11
0.9	0.19481E+01	-0.36342E+02	0.94753E+03	-0.27546E+05
	-0.18936E+01	0.46523E+01	-0.61444E+02	0.12087E+04
1.0	0.17572E+01	-0.57609E+00	0.29610E+00	-0.16776E+00
	-0.41096E-03	0.69606E-01	-0.18352E-01	0.70108E-02
Table 2D	Parameter =	4.00000 = λ		
	Period =	10.20329 = T		
	Floquet Exponent =	5.61746 = μ		
	Step Size = Period/	400		

TABLE 3

NUMERICAL EVALUATION OF ASYMPTOTIC PHASE FOR POINTS ON THE APPROXIMATE ISOCHRONS CALCULATED FOR

$$\dot{u} = -v + \lambda u \left(1 - \frac{u^3}{3}\right)$$
$$\dot{v} = u$$

(The phase difference at t = 5T would be almost 0 if the isochrons were exact.)

λ	φ	ε	Ischron Point u(ε)	v(ε)	Phase difference (after 5T) in units of T	Absolute Distance
		-1.0	2.7780	- .3250	.00261	.033
		- .5	2.2950	- .0101	.00128	.016
	0	+ .5	1.7649	.0035	.00117	.015
.5		+1.0	1.5838	.0060	.00227	.029
		-1.0	-1.4556	3.0281	.00392	.057
		- .5	- .8112	2.3686	.00150	.022
	.3T	+ .5	- .3579	1.7458	.00222	.032
		+1.0	- .1730	1.5213	.01151	.167
		-1.0	2.8068	- .0710	.00410	.054
		- .5	2.2582	- .0244	.00214	.028
	0	+ .5	1.6996	.0117	.00207	.027
1.0		+1.0	1.5088	.0202	.00432	.057
		-0.4	-1.3619	2.7314	.00197	.034
		-0.2	- .7322	2.3638	.00311	.053
	.3T	+0.2	- .2459	1.9862	.00314	.054
		+0.4	- .0582	1.8463	.01081	.184

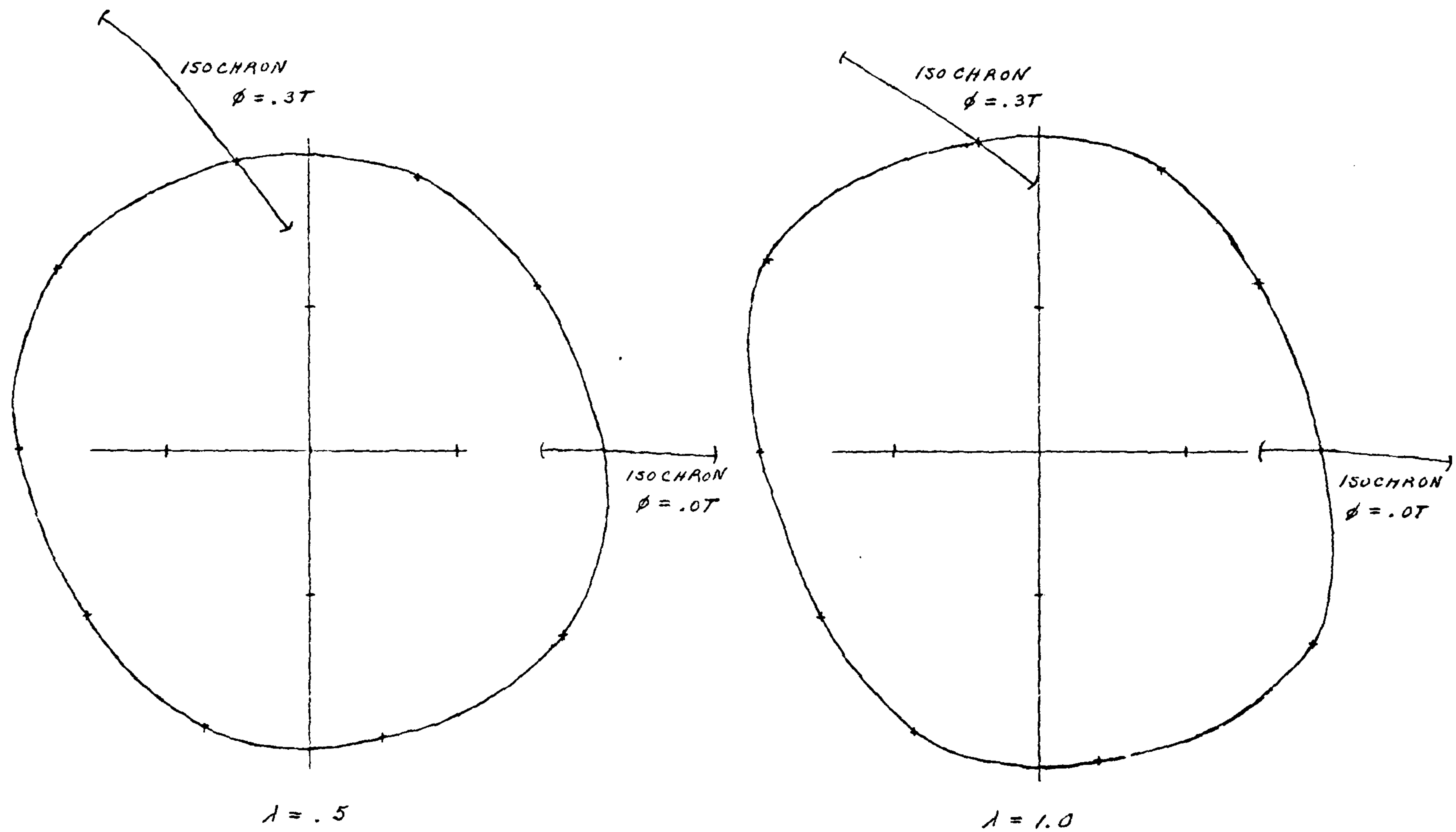


FIGURE 4. NUMERICALLY CALCULATED ISOCHRONS (BASED ON THE $\mathcal{O}(\epsilon^3)$ APPROXIMATION) WITH LIMIT CYCLES FOR THE VAN DER POL OSCILLATOR WITH $\lambda = .5, 1.0$: $u' = -v + \lambda(1 - u^2/3)$, $v' = u$. (TO SCALE, MARKED AT INTERVALS OF .1T.)

corners of the limit cycle). Since the expansion is convergent in (as shown in Appendix II), these larger coefficients show the radius of convergence is dropping rapidly to 0 near the corners. (In fact, for $\lambda = 10$, values of the fourth coefficients U_3, V_3 at

$\phi = .3T, .8T$ are $\sim 10^{30}$.)

This numerical work indicates the expansion (2.13) gives a reasonable approximation to the isochron near a smooth limit cycle, but that the radius of convergence (in ϵ) of the expansion becomes impractically small for "discontinuous" limit cycles.

CHAPTER IV

PERTURBATION OF THE LIMIT CYCLE SOLUTION TO REACTION-DIFFUSION EQUATIONS

Introduction

This chapter and the next study in detail the spatially perturbed limit cycle $(U(t),V(t))$ as a solution of the reaction-diffusion system

$$u_t = F(u,v) + (1+\alpha)\nabla_x^2 u, \tag{1.1}$$

$$v_t = G(u,v) + (1-\alpha)\nabla_x^2 v, \quad |\alpha| \leq 1,$$

where ∇_x is the gradient with respect to space variables $\underset{\sim}{x}$. The limit cycle is assumed to be kinetically stable and to have period T. This chapter is concerned with a perturbation approach using the idea of multiple scales: a spatial perturbation with a long space scale will be introduced with length dependent on a parameter ϵ, $0 < \epsilon \ll 1$. It is natural to couple this long spatial scale with changes ococurring on a slow time scale compared with the normal time scale T-periodic oscillation of the limit cycle. It is convenient to write the spatial scaling as $\underset{\sim}{\xi} = \sqrt{\epsilon}\,\underset{\sim}{x}$; choosing the slow time scale as $\tau = \epsilon t$, the $O(\epsilon)$-term of the perturbation contains both time and space effects. The basic result is a formal solution

$$u = U(t + \phi_0(\tau,\underset{\sim}{\xi}) + O(\epsilon)) + O(\epsilon),$$

$$v = V(t + \phi_0(\tau,\underset{\sim}{\xi}) + O(\epsilon)) + O(\epsilon).$$

where $U(t)$, $V(t)$ is the limit cycle.

This approach has been used by Neu (1979) in the case of a scalar diffusion matrix ($\alpha = 0$). Essentially, he obtained equation (2.2b.1) below for ϕ_0 and pointed out the existence of (unbounded) traveling wave solutions for ϕ_0, which he related to chemical waves propagating through a tube connecting two chemically oscillating solutions. Howard and Kopell (1977) have also obtained equation (2.2b.1) and the same (unbounded) traveling wave solution for ϕ_0 in the context of "weak shocks," transitions from one periodic traveling wave to a second one.

Here we are only concerned with cases in which the initial data for ϕ_0 (and all other functions) are bounded, in fact, periodic. The basic result is the determination of an "asymptotic phase" for the perturbed limit cycle solution.

Multiple scaling approaches (involving a slow time scale $\tau = \epsilon t$) are typically expected to be valid only over periods of time such that τ remains $O(1)$, that is, for normal time intervals $t \sim O(1/\epsilon)$. It may seem surprising in this context to speak of an "asymptotic phase," which can only refer to behavior occurring as $t \to +\infty$. However, it happens that the perturbed solutions considered here tend to decay to a spatially homogeneous solution as $t \to +\infty$. If the perturbation is dying away, there is no reason for the multi-scaling description to become less valid as time increases. (In fact, the numerical work of Chapter V shows it to represent the qualitative and quantitative behavior of the solutions as $t \to +\infty$.) Both Neu (1979) and Howard and Kopell (1977) were concerned with spatial dependence which persisted in time and the usual $O(1/\epsilon)$ restriction is to be expected in such cases.

Section 2 discusses the multiple scaling procedure and gives the expansion used, summarizes the results obtained in Section 2 and in Appendix III on the terms of the expansion, and also gives the traveling wave solution obtained by Neu (1979) and by Howard and Kopell (1977). The terms of the expansion through $O(\epsilon)$ are completely obtained (which requires that the $O(\epsilon^2)$ terms be almost completely obtained). Appendix II gives a recursion procedure for obtaining higher-order terms and shows that the expansion can be defined in such a way that the general terms have a reasonably simple form (given in (2.2c)). The original motivation for this detailed study was the hope of obtaining rigorous results on the asymptoticity (or convergence) of the expansion for small ϵ. Unfortunately, no such rigorous results could be obtained; remainder terms were always extremely complicated and no bounds could be derived. Instead, the validity of the expansion was studied by finding the behavior of the leading-order terms and making detailed predictions for the behavior of the actual solution.

Section 3 studies the leading-order terms of the expansion and makes such predictions. For the expansion through $O(\epsilon)$ (here ξ is a single space variable),

$$u = U(t + \phi_0(\tau,\xi) + \epsilon\,\phi_1(\tau,\xi) + O(\epsilon^2)) + \epsilon u_1 + O(\epsilon^2),$$

$$v = V(t + \phi_0(\tau,\xi) + \epsilon\,\phi_1(\tau,\xi) + O(\epsilon^2)) + \epsilon v_1 + O(\epsilon^2),$$

it is found that with periodic initial data, ϕ_0 and ϕ_1 converge to constants and u_1 and v_1 converge to 0 as $t \to +\infty$. From the behavior of the leading terms, the solution can be expected to evolve to a spatially homogeneous oscillation:

$$u = U(t + \hat{\phi}),$$

$$v = V(t + \hat{\phi}), \quad \hat{\phi} \text{ constant.}$$

Three predictions--concerning the independence of $\hat{\phi}$ on certain initial data, the rate of decay to the spatially homogeneous solution, and the value of $\hat{\phi}$--are made. These predictions are checked in Chapter V against numerical solutions for two specific reaction-diffusion systems.

Appendix IV gives an alternative multiple scaling approach. It is only partially studied because the equation governing the $O(\epsilon)$ behavior ((App. IV.1d) for A_1) cannot be solved explicitly as can the corresponding equation in section 2 ((2.2b.1) for ϕ_1).

A Formal Expansion Based on Multiple Scales

We wish to investigate solutions which correspond to perturbed limit cycle solutions of the reaction-diffusion system (1.1). It seems reasonable to consider effects involving three scales: a normal time scale (θ) for oscillations of the limit cycle, a slow time scale (τ) for effects occurring over many oscillations, and a long spatial scale ($\underset{\sim}{\xi}$) for slow spatial changes that do not represent an abrupt change from the spatially homogeneous limit cycle.

The method of multiple scales writes solutions in terms of these new variables $u = u(\theta,\tau,\underset{\sim}{\xi})$, $v = v(\theta,\tau,\underset{\sim}{\xi})$, and constructs $\theta,\tau,\underset{\sim}{\xi}$ as functions of t,x so that u,v satisfy the original reaction-diffusion system (1.1). The relations between $\theta,\tau,\underset{\sim}{\xi}$ are usually found by an expansion in ϵ. Let $0 < \epsilon << 1$ be a measure of slowness (of time or spatial change) and set

$$\tau = \epsilon t, \quad \underset{\sim}{\xi} = \sqrt{\epsilon}\, \underset{\sim}{x}, \quad \theta = t + \phi(\epsilon,\tau,\underset{\sim}{\xi}) = t + \sum_{n=0}^{\infty} \phi_n(\tau,\underset{\sim}{\xi})\epsilon^n.$$

Here $\tau,\underset{\sim}{\xi}$ are related to $t,\underset{\sim}{x}$ in a very simple way; the problem is to determine $\phi(\epsilon,\tau,\underset{\sim}{\xi})$. The scalings have been chosen so that the scaled temporal and spatial derivative terms $\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial \tau}$, $\nabla_x^{\,2} = \epsilon \nabla_\xi^2$ are of the same order. If only $\underset{\sim}{x}$ is scaled, then (1.1) becomes

$$u_t = F(u,v) + (1+\alpha)\,\epsilon\,\nabla_\xi^2\, u,$$

$$v_t = G(u,v) + (1-\alpha)\,\epsilon\,\nabla_\xi^2\, v,$$

which can be interpreted as $O(\epsilon)$-diffusion coefficients and $O(1)$ changes in ξ-space. (This form of the reaction-diffusion system is that used in the numerical calculations of Chapter V).

The u,v functions are expanded in terms of ϵ :

$$\begin{bmatrix} u \\ v \end{bmatrix} = \sum_{n=0}^{\infty} \begin{bmatrix} u_n(\theta,\tau,\xi) \\ v_n(\theta,\tau,\xi) \end{bmatrix} \epsilon^n. \tag{2.1b}$$

The equations (1.1) become (here and for the rest of the chapter $\nabla \equiv \nabla_3$):

$$(1+\epsilon\phi_\tau)\begin{bmatrix} u_\theta \\ v_\theta \end{bmatrix} + \epsilon\begin{bmatrix} u_\tau \\ v_\tau \end{bmatrix} = \begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} \tag{2.1c}$$

$$+ \ \epsilon \begin{bmatrix} (1+\alpha)(\nabla^2 u + u_\theta \nabla^2\phi + 2\nabla\phi\cdot\nabla u + |\nabla\phi|^2 u_{\theta\theta}) \\ (1-\alpha)(\nabla^2 v + v_\theta \nabla^2\phi + 2\nabla\phi\cdot\nabla v + |\nabla\phi|^2 v_{\theta\theta}) \end{bmatrix} .$$

To expand the equation as a power series in ϵ, it is necessary to expand $F(u,v)$, $G(u,v)$ as power series in ϵ. This procedure has already been used in Chapter III, so the notation and properties in (III.2.5a-c) are used here.

$$\sum_{n=0}^{\infty} \begin{bmatrix} u_{n\theta} \\ v_{n\theta} \end{bmatrix} \epsilon^n = \begin{bmatrix} F(u_o, v_o) \\ G(u_o, v_o) \end{bmatrix} + \sum_{n=1}^{\infty} \begin{bmatrix} F_u(u_o, v_o) & F_v(u_o, v_o) \\ G_u(u_o, v_o) & G_v(u_o, v_o) \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} \epsilon^n$$

$$+ \sum_{n=2}^{\infty} \begin{bmatrix} F_n(u_o, \ldots, u_{n-1}, v_o, \ldots, v_{n-1}) \\ G_n(u_o, \ldots, u_{n-1}, v_o, \ldots, v_{n-1}) \end{bmatrix} \epsilon^n \tag{2.1d}$$

$$+ \sum_{n=0}^{\infty} \left[\begin{array}{l} -u_{n\tau} + (1+\alpha)\nabla^2 u_n + \sum\limits_{k+\ell=n} (u_{k\theta}(-\phi_{\ell\tau} + (1+\alpha)\nabla^2\phi_\ell) \\ -v_{n\tau} + (1-\alpha)\nabla^2 v_n + \sum\limits_{k+\ell=n} (u_{k\theta}(-\phi_{\ell\tau} + (1-\alpha)\nabla^2\phi_\ell) \end{array} \right.$$

$$\left. \begin{array}{l} + 2(1+\alpha)\nabla u_k \cdot \nabla\phi_\ell \;) + \sum\limits_{k+\ell+m=n} (1+\alpha) u_{k\theta\theta} \nabla\phi_\ell \cdot \nabla\phi_m \\ + 2(1-\alpha)\nabla v_k \cdot \nabla\phi_\ell \;) + \sum\limits_{k+\ell+m=n} (1-\alpha) v_{k\theta\theta} \nabla\phi_\ell \cdot \nabla\phi_m \end{array} \right] \epsilon^n .$$

Equating the coefficients of the $O(\epsilon^n)$ - terms in (2.1d) generates an infinite family of equations for u_n, v_n, ϕ_n. Each $O(\epsilon^n)$ term yields only a pair of equations, which determine the θ-dependence of u_n, v_n but leave the $\tau, \underset{\sim}{\xi}$ dependence only partially determined. The ϕ_n are determined by boundedness conditions on the u_n, v_n, and other conditions are imposed to completely specify the $\tau, \underset{\sim}{\xi}$ dependence of u_n, v_n.

Since the calculations of this section and Appendix III are messy it will be helpful to state at this point precisely what results are obtained and the order in which they arise. The main problem is to obtain equations and initial conditions for all terms u_n, v_n, ϕ_n, specifying these variables in a reasonable way. The structure of the terms u_n, v_n will be considered first; the relevant initial conditions are then more easily described.

First, it is obvious that the $O(1)$-term in (2.1d) has the solution

$$\begin{bmatrix} u_o \\ v_o \end{bmatrix} = \begin{bmatrix} U(\theta) \\ V(\theta) \end{bmatrix} , \qquad (2.2a)$$

which is a reasonable choice since we are perturbing the limit cycle. To obtain the higher-order terms, we need the solutions of the variational equation of the kinetic system about the limit cycle, given in Lemma C of Appendix I; the fundamental matrix is written as

$$\begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U}(t) \\ V'(t) & \exp(-\mu t)\hat{V}(t) \end{bmatrix} ,$$

where U', V', $\hat{U}$, $\hat{V}$ are T-periodic functions and $-\mu$ is the negative Floquet exponent. From a consideration of the $O(\epsilon)$-term, it will be shown below that u_1, v_1 will contain terms growing like $O(\theta)$ unless ϕ_o satisfies a certain equation. Deleting these $O(\theta)$-terms gives:

(1) $\phi_{o\tau} = (1 + \alpha h_1)\nabla^2\phi_o + (\ell_1 + \alpha m_1)|\nabla\phi_o|^2$;

(2) the constants h_1, ℓ_1, m_1 are given by (2.5) below; (2.2b)

(3) $$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \begin{bmatrix} P_{10}(\tau,\underset{\sim}{\xi},\theta) \\ Q_{10}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} + \exp(-\mu\theta)\ (B_1(\tau,\underset{\sim}{\xi}) + f(\tau,\underset{\sim}{\xi})\ \begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix} ;$$

(4) $P_{10}(\tau,\underset{\sim}{\xi},\theta)$, $Q_{10}(\tau,\underset{\sim}{\xi},\theta)$ are linear combinations of T-periodic functions of θ with coefficients which are polynomials in $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau,\underset{\sim}{\xi})$ and functions of $\phi_o(0,\underset{\sim}{\xi})$; $f(\tau,\underset{\sim}{\xi})$ is a linear combination of $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau,\underset{\sim}{\xi})$; in particular, if the $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau,\underset{\sim}{\xi})$ go to 0 as $\tau\to+\infty$, then P_{10}, Q_{10}, $f\to 0$ as $\tau\to+\infty$;

(5) $B_1(\tau,\underset{\sim}{\xi})$ is a function arising from the solution of an ODE in θ for u_1,v_1 (and determined from $O(\epsilon^2)$ terms).

The equation for ϕ_o is a form of Burgers' equation and can be solved exactly by a transformation to the heat equation--this solution is discussed in Section 3.

The solution for u_2, v_2 will be given in detail, partly because the detail is necessary in obtaining the equation for B_1 and partly because the calculations are slightly different from those for u_n, v_n, $n \geq 3$. In the solution for u_2, v_2, two notable types of terms occur. The first type of term grows like θ and their elimination gives a condition on ϕ_1. The second type contains the product $\theta \exp(-\mu \theta)$. The $O(\theta)$ terms are eliminated to retain bounded solutions, but this reason does not apply to terms containing $\theta \exp(-\mu \theta)$ since these remain bounded as $\theta \to +\infty$. However, since all terms occurring are either periodic in θ or a product of $\exp(-\mu\theta)$ or $\theta \exp(-\mu\theta)$ and a periodic function of θ, and since the $\theta \exp(-\mu\theta)$ terms will lead to terms involving $\theta^n \exp(-\mu\theta)$ at higher orders if left in, it seems obvious we should eliminate the $\theta \exp(-\mu\theta)$ quantities. In fact, this procedure yields an equation for B_1, which is exactly what is needed.

The material in (2.2a,b) and (2.2c) with $n=2$ is derived in this section. In Appendix III we use an induction argument to study the coefficients of ϵ^n for $n \geq 3$. Altogether (for $n \geq 2$),

(1) deleting terms in u_n, v_n containing θ leads to a linear inhomogeneous equation for ϕ_{n-1}, (2.2c)

$$\phi_{n-1,\tau} = (1 + \alpha h_1)\nabla^2 \phi_{n-1} + 2(\ell_1 + \alpha m_1)\nabla\phi_0 \cdot \nabla\phi_{n-1} + h_{n-1}(\tau, \underset{\sim}{\xi});$$

(2) $h_{n-1}(\tau, \underset{\sim}{\xi})$ is a polynomial in the $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau, \underset{\sim}{\xi})$, $\ldots, \phi_{n-2}(\tau, \underset{\sim}{\xi})$ and functions of $\phi_0(0, \underset{\sim}{\xi})$; in particular, if the $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau, \underset{\sim}{\xi})$, $\ldots$, $\phi_{n-2}(\tau, \underset{\sim}{\xi})$ go to 0 as $\tau \to +\infty$, then $h_{n-1}(\tau, \underset{\sim}{\xi}) \to 0$ as $\tau \to +\infty$;

(3) deleting terms in u_n, v_n containing $\theta\exp(-\mu\theta)$ leads to a linear inhomogeneous equation for B_{n-1}, $n \geq 3$,

$$B_{n-1,\tau} = (1 - \alpha h_1)\nabla^2 B_{n-1} + 2(\ell_{21} + \alpha\ell_{22} - \mu(1 - \alpha h_1))\nabla\phi_o \cdot \nabla B_{n-1}$$

$$+ f_{n-1}(\tau, \underset{\sim}{\xi}) B_{n-1} + \hat{h}_{n-1}(\tau, \underset{\sim}{\xi}),$$

and for $n=2$ and $\hat{B} = B_1(\tau, \underset{\sim}{\xi}) + f(\tau, \underset{\sim}{\xi})$,

$$\hat{B}_\tau = (1 - \alpha h_1)\nabla^2\hat{B} + 2(\ell_{21} + \alpha\ell_{22}$$

$$-\mu(1 - \alpha h_1))\nabla\phi_o \cdot \nabla\hat{B} + f_1(\tau, \underset{\sim}{\xi})\hat{B}.$$

(4) $f_{n-1}(\tau, \underset{\sim}{\xi})$ is a polynomial in $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau, \underset{\sim}{\xi})$, ..., $\phi_{n-2}(\tau, \underset{\sim}{\xi})$ and functions of $\phi_o(0, \underset{\sim}{\xi})$ such that $f_{n-1} \to 0$ as $\tau \to +\infty$ if the $\underset{\sim}{\xi}$-derivatives of ϕ_o, ..., $\phi_{n-2} \to 0$; $\hat{h}_{n-1}(\tau, \underset{\sim}{\xi})$ depends on ϕ_o, ..., ϕ_{n-2} and B_1, ..., B_{n-2}.

(5) $$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = B_n(\tau, \underset{\sim}{\xi}) \exp(-\mu\theta) \begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix}$$

$$+ \sum_{k=0}^{n} \exp(-k\mu\theta) \begin{bmatrix} P_{nk}(\tau, \underset{\sim}{\xi}, \theta) \\ Q_{nk}(\tau, \underset{\sim}{\xi}, \theta) \end{bmatrix} ;$$

(6) each P_{nk}, Q_{nk} is a linear combination of T-periodic functions of θ such that each coefficient is a polynomial in $B_1, \ldots, B_{n-1}$ and their $\underset{\sim}{\xi}$-derivatives, the $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau,\underset{\sim}{\xi}), \ldots, \phi_{n-1}(\tau,\underset{\sim}{\xi})$, and functions of $\phi_o(0,\underset{\sim}{\xi})$; in particular, the coefficients in P_{n0}, Q_{n0} do not contain $B_1, \ldots, B_{n-1}$ or their derivatives, but depend on the $\underset{\sim}{\xi}$-derivatives of $\phi_o'(\tau,\underset{\sim}{\xi}), \ldots, \phi_{n-1}(\tau,\underset{\sim}{\xi})$ and if these go to zero as $\tau \to +\infty$, then $P_{no}, Q_{no} \to 0$ as $\tau \to +\infty$.

(7) $B_n(\tau,\underset{\sim}{\xi})$ is a function arising from the solution of an ODE in θ for u_n, v_n (and determined from the $O(\epsilon^{n+1})$ term). We note that the equation for ϕ_{n-1} can be transformed into the heat equation. The detailed behavior of ϕ_1 and B_1 are studied in section 3.

Initial conditions are taken as

$$\begin{aligned} &\phi_o(0,\underset{\sim}{\xi}) \text{ arbitrary}, \quad \phi_n(0,\underset{\sim}{\xi}) \equiv 0 \text{ for } n \geq 1, \\ &B_1(0,\underset{\sim}{\xi}) \text{ arbitrary}, \quad B_n(0,\underset{\sim}{\xi}) \equiv 0 \text{ for } n \geq 2, \end{aligned} \tag{2.3}$$

corresponding to initial data for u,v of the form

$$\begin{bmatrix} u(0,\underset{\sim}{\xi}) \\ v(0,\underset{\sim}{\xi}) \end{bmatrix} = \begin{bmatrix} U(\phi_o(0,\underset{\sim}{\xi})) \\ V(\phi_o(0,\underset{\sim}{\xi})) \end{bmatrix} + B_1(0,\underset{\sim}{\xi}) \exp(-\mu\phi_o(0,\underset{\sim}{\xi}))$$

$$\begin{bmatrix} \hat{U}(\phi_o(0,\underset{\sim}{\xi})) \\ \hat{V}(\phi_o(0,\underset{\sim}{\xi})) \end{bmatrix} .$$

In connection with the initial conditions the experience of Chapter III should be noted. There an exceptionally simple form (III.2.8) of the terms in the expansion for solutions near the limit cycle was found. That simple form, however, forced a particular choice of initial conditions for each term (III.2.13). This fact suggests that an expansion simpler than (2.2) may arise but at the cost of more complex initial conditions. Unfortunately, considerable search and experimentation has not produced any particular simplification in (2.2), so the simple initial conditions (2.3) have been kept.

Both Neu (1979) and Howard and Kopell (1977) point out the existence of a "weak shock" solution for ϕ_o. Specifically, if equation (2.2b.1) is written in the form (ξ = single space variable)

$$p_\tau = p_{\xi\xi} - \frac{k}{2} p_\xi^2 ,$$

then p_ξ solves Burgers' equation

$$q_\tau = q_{\xi\xi} - k\, q\, q_\xi ,$$

with traveling wave solutions $(q_1, q_2$ constants)

$$q = q_1 + \frac{q_2 - q_1}{1 + \exp\left(\frac{k}{2}(q_2 - q_1)\left(\xi - \frac{k}{2}(q_1 + q_2)\tau\right)\right)}$$

$$\sim q_1, q_2 \quad \text{as} \quad \xi \to \pm\infty.$$

Consequently, a "weak shock" solution of the form

$$\begin{bmatrix} u \\ v \end{bmatrix} \sim \begin{bmatrix} U(t + p(\xi - \frac{k}{2}(q_2 + q_1)\tau) \\ V(t + p(\xi - \frac{k}{2}(q_2 + q_1)\tau) \end{bmatrix},$$

$$p(\xi) = \int_0^\xi (q_1 + \frac{q_2 - q_1}{1 + \exp(\frac{k}{2}(q_2 - q_1)s)})\, ds$$

$$\sim q_1 \xi \;, q_2 \xi \quad \text{as} \quad \xi \to \pm\infty,$$

is assumed to exist. The resulting solution is essentially one traveling wave with spatial wavelength $T/q_1\sqrt{\epsilon}$ attached to another traveling wave with wavelength $T/q_2\sqrt{\epsilon}$, and the two moving together with speed (in x,t coordinates) $\frac{k}{2}(q_2 + q_1)\sqrt{\epsilon}$.

Here we are only concerned with bounded functions ϕ_o and will assume ϕ_o is periodic in $\underset{\sim}{\xi}$.

We now proceed with the proof of (2.2b-c). To calcuate u_1, v_1, the coefficient of ϵ in (2.1d) is

$$\begin{bmatrix} u_{1\theta} \\ v_{1\theta} \end{bmatrix} = \begin{bmatrix} F_u(U,V) & F_v(U,V) \\ G_u(U,V) & G_v(U,V) \end{bmatrix} \begin{bmatrix} u_1 \\ v_1 \end{bmatrix} \tag{2.4}$$

$$+ \begin{bmatrix} (-\phi_{o\tau} + (1+\alpha)\nabla^2\phi_o)U'(\theta) + (1+\alpha)|\nabla\phi_o|^2 U''(\theta) \\ (-\phi_{o\tau} + (1-\alpha)\nabla^2\phi_o)V'(\theta) + (1-\alpha)|\nabla\phi_o|^2 V''(\theta) \end{bmatrix}.$$

Lemma D of Appendix I gives the general solution. Define

$$\int_0^{\theta} \begin{bmatrix} \hat{V}(s) & -\hat{U}(s) \\ -\exp(\mu s)V'(s) & \exp(\mu s)U'(s) \end{bmatrix} \begin{bmatrix} U'(s) & U'(s) & U''(s) & -U''(s) \\ V'(s) & -V'(s) & V''(s) & -V''(s) \end{bmatrix}$$

$$\frac{ds}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)} \tag{2.5}$$

$$= \begin{bmatrix} \theta & h_1(\theta)+H_1(\theta) & \ell_1\theta+L_1(\theta) & m_1\theta+M_1(\theta) \\ 0 & \hat{h}_1+\exp(\mu\theta)\hat{H}_1(\theta) & \hat{\ell}_1+\exp(\mu\theta)\hat{L}_1(\theta) & \hat{m}_1+\exp(\mu\theta)\hat{M}_1(\theta) \end{bmatrix},$$

where H_1, L_1, M_1, $\hat{H}_1$, $\hat{L}_1$, $\hat{M}_1$ are all T-periodic functions of 0 by Lemma A. The general solution can now be written as:

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = A_1(\tau,\underset{\sim}{\xi}) \begin{bmatrix} U'(\theta) \\ V'(\theta) \end{bmatrix} + B_1(\tau,\underset{\sim}{\xi})\exp(-\mu\theta) \begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix}$$

$$+ \begin{bmatrix} U'(s) & \exp(\mu s)\hat{U}(s) \\ V'(s) & \exp(\mu s)\hat{V}(s) \end{bmatrix} \Bigg((-\phi_{0\tau} + \nabla^2\phi_0) \begin{bmatrix} s \\ 0 \end{bmatrix} \tag{2.6a}$$

$$+\alpha\nabla^2\phi_0 \begin{bmatrix} h_1 s + H_1(s) \\ \hat{h}_1 + \exp(\mu s)\hat{H}_1(s) \end{bmatrix} + |\nabla\phi_0|^2 \begin{bmatrix} \ell_1 s + L_1(s) \\ \hat{\ell}_1 + \exp(\mu s)\hat{L}_1(s) \end{bmatrix}$$

$$+\alpha|\nabla\phi_0|^2 \begin{bmatrix} m_1 s + M_1(s) \\ \hat{m}_1 + \exp(\mu s)\hat{M}_1(s) \end{bmatrix} \Bigg) \Bigg|_{\hat{\theta}}^{\theta},$$

where the initial value $\hat{\theta} = \phi_o(0,\underset{\sim}{\xi})$ is obtained from (2.3). The (2.2b.1,2) for ϕ_o follows by requiring the $O(\theta)$ terms to cancel out. We set $A_1(\tau,\underset{\sim}{\xi}) \equiv 0$* -- this requirement could lead to trouble by introducing secular behavior in higher-order terms, but it will be shown below and in Appendix III that no such difficulty occurs. The solution reduces to

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = B_1(\tau,\underset{\sim}{\xi})\exp(-\mu\theta)\begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix} \tag{2.6b}$$

$$+\Bigg(\left(\alpha\nabla^2\phi_o\, H_1(s) + |\nabla\phi_o|^2\,(L_1(s) + \alpha M_1(s))\right)\begin{bmatrix} U'(s) \\ V'(s) \end{bmatrix}$$

$$+\left(\alpha\nabla^2\phi_o\,\hat{H}_1(s) + |\nabla\phi_o|^2(\hat{L}_1(s) + \alpha\hat{M}_1(s))\right)\begin{bmatrix} \hat{U}(s) \\ \hat{V}(s) \end{bmatrix}\Bigg)\Bigg|_{\hat{\theta}}^{\theta}$$

$$+\left(\exp(-\mu s)\,(\alpha\nabla^2\phi_o\,\hat{h}_1 + |\nabla\phi_o|^2(\hat{\ell}_1 + \alpha\hat{m}_1))\begin{bmatrix} \hat{U}(s) \\ \hat{V}(s) \end{bmatrix}\right)\Bigg|_{\hat{\theta}}^{\theta}.$$

*The possibility of keeping A_1 and deriving an equation for it (in place of ϕ_1) is explored in Appendix IV.

The definitions of P_{10}, Q_{10}, f and (2.2b.3, 4, 5) follow immediately by *inspection (the terms evaluated at* $\hat{\theta} = \phi_o(0,\underset{\sim}{\xi})$ are included in the periodic term).

For the calculation of u_2, v_2, the coefficient of ϵ^2 is

$$\begin{bmatrix} u_{2\theta} \\ v_{2\theta} \end{bmatrix} = \begin{bmatrix} F_u(U,V) & F_v(U,V) \\ G_u(U,V) & G_v(U,V) \end{bmatrix} \begin{bmatrix} u_2 \\ v_2 \end{bmatrix} \tag{2.7}$$

$$+ \begin{bmatrix} (-\phi_{1\tau} + (1+\alpha)\nabla^2\phi_1)U'(\theta) + 2(1+\alpha)\nabla\phi_o\cdot\nabla\phi_1 \; U''(\theta) \\ (-\phi_{1\tau} + (1-\alpha)\nabla^2\phi_1)V'(\theta) + 2(1-\alpha)\nabla\phi_o\cdot\nabla\phi_1 \; V''(\theta) \end{bmatrix}$$

$$+ \begin{bmatrix} -u_{1\tau} - \phi_{o\tau}u_{1\theta} + (1+\alpha)(\nabla^2 u_1 + \nabla^2\phi_o u_{1\theta} + 2\nabla\phi_o\cdot\nabla u_{1\theta} \\ \qquad + u_{1\theta\theta}|\nabla\phi_o|^2) \\ -v_{1\tau} - \phi_{o\tau}v_{1\theta} + (1-\alpha)(\nabla^2 v_1 + \nabla^2\phi_o v_{1\theta} + 2\nabla\phi_o\cdot\nabla v_{1\theta} \\ \qquad + v_{1\theta\theta}|\nabla\phi_o|^2) \end{bmatrix}$$

(term # 1)

$$+ \begin{bmatrix} F_2(u_o,u_1,v_o,v_1) \\ G_2(u_o,u_1,v_o,v_1) \end{bmatrix} \quad \text{(term \#2)},$$

where $F_2 = \frac{1}{2}\left[F_{uu}(u_o,v_o)u_1^2 + 2\,F_{uv}(u_o,v_o)u_1v_1 + F_{vv}(u_o,v_o)v_1^2\right]$,

and similarly for G_2.

First expand terms #1 and #2 into powers of $\exp(-\mu\theta)$ and then expand further to obtain the $\hat{B}$-dependence ($\hat{B} = B_1(\tau,\underset{\sim}{\xi}) + f(\tau,\underset{\sim}{\xi})$ giving:

$$
\begin{aligned}
(\text{Term \#1}) + (\text{Term \#2}) = &\begin{bmatrix} R_{10}(\tau,\underset{\sim}{\xi},\theta) \\ \\ S_{10}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} + \exp(-2\mu\theta)\hat{B}^2 \begin{bmatrix} R_{12}(\tau,\underset{\sim}{\xi},\theta) \\ \\ S_{12}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} \\
+ \exp(-\mu\theta) &\left[\begin{array}{l}
\Big(-\hat{B}_\tau + \mu\phi_{o\tau}\hat{B} + (1+\alpha)(\nabla^2\hat{B} - \mu\nabla^2\phi_o\hat{B} - 2\mu\nabla\phi_o\cdot\nabla\hat{B} \\
+ \mu^2|\nabla\phi_o|^2\hat{B})\Big)\hat{U} + \Big(-\phi_{o\tau}\hat{B} + (1+\alpha)(\nabla^2\phi_o\hat{B} \\
+ 2\nabla\phi_o\cdot\nabla\hat{B} - 2\mu|\nabla\phi_o|^2\hat{B})\Big)\hat{U}' + (1+\alpha)|\nabla\phi_o|^2\hat{B}\,\hat{U}'' \\
+ R_{11}(\tau,\underset{\sim}{\xi},\theta)\hat{B} \\
\Big(-\hat{B}_\tau + \mu\phi_{o\tau}\hat{B} + (1-\alpha)(\nabla^2\hat{B} - \mu\nabla^2\phi_o\hat{B} \\
- 2\mu\nabla\phi_o\cdot\nabla\hat{B} + \mu^2|\nabla\phi_o|^2\hat{B})\Big)\hat{V} + \Big(-\phi_{o\tau}\hat{B} + (1-\alpha) \\
(\nabla^2\phi_o\hat{B} + 2\nabla\phi_o\cdot\nabla\hat{B} - 2\mu|\nabla\phi_o|^2\hat{B})\Big)\hat{V}' + \\
(1-\alpha)|\nabla\phi_o|^2\hat{B}\,\hat{V}'' + S_{11}(\tau,\underset{\sim}{\xi},\theta)\hat{B}
\end{array}\right]
\end{aligned}
\tag{2.8}
$$

where $R_{1k}(\tau,\underset{\sim}{\xi},\theta)$, $S_{1k}(\tau,\underset{\sim}{\xi},\theta)$, k = 0, 1, 2, are linear combinations of T-periodic functions of θ with coefficients which are polynomials in $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau,\underset{\sim}{\xi})$ and functions of $\phi_o(0,\underset{\sim}{\xi})$; these polynomials are such that R_{1k}, $S_{1k} \to 0$ as $\tau \to +\infty$ if the $\underset{\sim}{\xi}$-derivatives of $\phi_o(\tau,\underset{\sim}{\xi}) \to 0$ as $\tau \to +\infty$.

Again, Lemma D of Appendix I will be used to express u_2, v_2

Define

$$\int_0^{\theta} \begin{bmatrix} \hat{V}(s) & -\hat{U}(s) \\ -\exp(\mu s)V'(s) & \exp(\mu s)U'(s) \end{bmatrix}$$

$$\begin{bmatrix} \hat{U}(s) & \hat{U}(s) & \hat{U}'(s) & \hat{U}'(s) & \hat{U}''(s) & \hat{U}''(s) \\ \hat{V}(s) & -\hat{V}(s) & \hat{V}'(s) & -\hat{V}'(s) & \hat{V}''(s) & -\hat{V}''(s) \end{bmatrix}$$

$$\frac{\exp(-\mu s)ds}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)} \tag{2.9}$$

$$= \begin{bmatrix} 0 & k_1 + \exp(-\mu\theta)K_1(\theta) & \hat{\ell}_{21} + \exp(-\mu\theta)\hat{L}_{21}(\theta) & \hat{\ell}_{22} + \exp(-\mu\theta)\hat{L}_{22}(\theta) & \hat{m}_{21} + \exp(-\mu\theta)\hat{M}_{21}(\theta) & \hat{m}_{22} + \exp(-\mu\theta)\hat{M}_{22}(\theta) \\ \theta & -h_1\theta - H_1(\theta) & \ell_{21}\theta + L_{21}(\theta) & \ell_{22}\theta + L_{22}(\theta) & m_{21}\theta + M_{21}(\theta) & m_{22}\theta + M_{22}(\theta) \end{bmatrix},$$

where K_1, L_{21}, $\hat{L}_{21}$, M_{21}, $\hat{M}_{21}$, L_{22}, $\hat{L}_{22}$, M_{22}, $\hat{M}_{22}$ are T-periodic functions of θ (using Lemma A). The general solution for u_2, v_2 can be written as:

$$\begin{bmatrix} u_2 \\ v_2 \end{bmatrix} = A_2(\tau,\underset{\sim}{\xi}) \begin{bmatrix} U'(\theta) \\ V'(\theta) \end{bmatrix} + B_2(\tau,\underset{\sim}{\xi}) \exp(-\mu\theta) \begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix}$$

$$+ \begin{bmatrix} (-\phi_{1\tau} + (1+\alpha h_1)\nabla^2\phi_1 + 2(\ell_1 + \alpha m_1)\nabla\phi_0 \cdot \nabla\phi_1 + h_1(\tau,\underset{\sim}{\xi}))\theta \\ (-\hat{B}_\tau + (1-\alpha h_1)\nabla^2\hat{B} + 2(\ell_{21} + \alpha\ell_{22} - \mu(1-\alpha h_1))\nabla\phi_0 \cdot \nabla\hat{B} \\ \quad + f_1(\tau,\underset{\sim}{\xi})\hat{B})\theta \exp(-\mu\theta) \end{bmatrix}$$

$$+ \begin{bmatrix} P_{20}(\tau,\underset{\sim}{\xi},\theta) \\ Q_{20}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} + \exp(-\mu\theta) \begin{bmatrix} P_{21}(\tau,\underset{\sim}{\xi},\theta) \\ Q_{21}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix}$$

$$+ \exp(-2\mu\theta) \begin{bmatrix} P_{22}(\tau,\underset{\sim}{\xi},\theta) \\ Q_{22}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} , \tag{2.10}$$

where

$$h_1(\tau,\underset{\sim}{\xi}) = \frac{1}{T}\int_0^T \frac{R_{10}(\tau,\underset{\sim}{\xi},s)\hat{V}(s) - S_{10}(\tau,\underset{\sim}{\xi},s)\hat{U}(s)}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)}\, ds,$$

$$f_1(\tau,\underset{\sim}{\xi}) = \frac{1}{T}\int_0^T \frac{U'(s)R_{11}(\tau,\underset{\sim}{\xi},s) - V'(s)S_{11}(\tau,\underset{\sim}{\xi},s)}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)}\, ds.$$

As before we set $A_2 \equiv 0$ (the next section shows this leads to no difficulties in the higher-order terms). The results (2.2.c) for n=2 are obtained as follows. The coefficient of θ is required to be 0 -- this yields (2.2c.1,2). The coefficient of $\theta \exp(-\mu\theta)$ is required to be 0 -- this yields (2.2c.3,4). The remaining terms, together with the properties of $R_{1k}(\tau,\underset{\sim}{\xi},\theta)$, $S_{1k}(\tau,\underset{\sim}{\xi},\theta)$ mentioned in connection with (2.8), yield (2.2c.5,6,7).

We have obtained (2.2a,b) and (2.2.c) for n=2; the remaining results in (2.2c) for $n \geq 3$ are obtained by induction in Appendix III.

Three Predictions of Solution Behavior

The multiple scaling expansion of Section 2 and Appendix III has been derived as a purely formal expansion--no proofs of convergence or asymptoticity have been obtained. Consequently we can only study its validity indirectly by making predictions of solution behavior based on the expansion and comparing these predictions with real (numerical) solutions. This section studies the behavior of the first two terms of the expansion:

$$\begin{bmatrix} u \\ v \end{bmatrix} \sim \begin{bmatrix} u_o(\theta) \\ v_o(\theta) \end{bmatrix} + \epsilon \begin{bmatrix} u_1(\tau,\underset{\sim}{\xi},\theta) \\ v_1(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} , \tag{3.1}$$

and makes predictions about the behavior of u,v which can be checked numerically. These checks are carried out in Chapter V.

One point on consistency with previous results should be mentioned first. Chapter II gives a condition for linear stability (instability) of the limit cycle to perturbations with small wave number k^2. Small wave numbers correspond to long wavelengths, which is the type of of spatial behavior considered in Section 2, so a relation between the expansion and Chapter II is to be expected. In fact, by Theorem II.1 the limit cycle is linearly stable (unstable) to small wave number perturbations if

$$1-\alpha A_o = 1 + \frac{\alpha}{T}\int_0^T \frac{U'(s)\hat{V}(s) + V'(s)\hat{U}(s)}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)}\, ds > 0 \quad (<0).$$

But $1-\alpha A_o = 1+\alpha h_1$ by (2.5), so the limit cycle is linearly stable or unstable depending on whether the coefficient of $\nabla^2\phi_o$ is positive or negative in (2.2b.1): $\phi_{0\tau} = (1+\alpha h_1)\nabla^2\phi_0 + \ldots$. (Incidentally, the equation (2.2c.3) for $\hat{B} = B_1(\tau,\underset{\sim}{\xi}) + f(\tau,\underset{\sim}{\xi})$ has the form $\hat{B}_\tau = (1-\alpha h_1)\nabla^2\hat{B} + \ldots$, and it is possible that $1+\alpha h_1 > 0$ and $1-\alpha h_1 < 0$. This situation has not been investigated here; $1\underline{+}\alpha h_1 > 0$ in the cases solved numerically in Chpater V.)

The work of this section will result in three predictions on the behavior of perturbed limit cycle solutions of (1.1):

Prediction I. Periodic initial data (period = P) in (2.3) should evolve to a spatially homogeneous solution of the form $(U(t+\hat{\phi}), V(t+\hat{\phi}))$, where (the asymptotic phase) $\hat{\phi}$ is a constant that is independent of $B_1(0,\underset{\sim}{\xi})$.

Prediction II. The amplitude of the perturbation to the limit cycle should decay like $\exp(-(1+\alpha h_1)\,(\frac{2\pi}{P})^2\,\epsilon\, t)$.

Prediction III. The asymptotic phase $\hat{\phi}$ can be approximated as

$$\hat{\phi} = \phi_0(+\infty) + O(\epsilon)$$

$$= \frac{1+\alpha h_1}{\ell_1+\alpha m_1}\,\ell n\left(\frac{1}{P}\int_0^P \exp\left(\frac{\ell_1+\alpha m_1}{1+\alpha h_1}\,\phi_0(0,\xi)\right)d\xi\right) + O(\epsilon).$$

In particular, if $\phi_0(0,\xi) = A\sin(\frac{2k\pi}{P}\,\xi)$, then

$$\hat{\phi} = \frac{1+\alpha h_1}{\ell_1+\alpha m_1}\,\ell n\left[I_o\left(A\left(\frac{\ell_1+\alpha m_1}{1+\alpha h_1}\right)\right)\right],$$

where $I_0(x)$ is the modified Bessel function.

These predictions result from the following study of the behavior of the leading-order terms (3.1) of the expansion.

We first show that equations (2.2b.1), (2.2c.1) for ϕ_n, $n \geq 0$, can be transformed to the heat equation. If $\ell_1 + \alpha m_1 = 0$, each ϕ_n already satisfies the heat equation; if $\ell_1 + \alpha m_1 \neq 0$, the following transformation, based on the Hopf-Cole transformation, can be made:

if $\quad \phi_{0\tau} = (1+\alpha h_1)\nabla^2\phi_0 + (\ell_1+\alpha m_1)|\nabla\phi_0|^2$ and $\psi_0 = \exp\left(\frac{\ell_1+\alpha m_1}{1+\alpha h_1}\phi_0\right)$,

then $\psi_{0\tau} = (1+\alpha h_1)\nabla^2\psi_0$,

if $\quad \phi_{n\tau} = (1+\alpha h_1)\nabla^2\phi_n + 2(\ell_1+\alpha m_1)\nabla\phi_0\cdot\nabla\phi_n + h_n(\tau,\underset{\sim}{\xi})$ and $\psi_n = \psi_0\phi_n$,

then $\psi_{n\tau} = (1+\alpha h_1)\nabla^2\psi_n + h_n(\tau,\underset{\sim}{\xi})$.

For simplicity we consider only periodic initial data in one space variable ξ; period = P. Lemma 1 gives the behavior of solutions to the heat equation required for the analysis of (3.1).

Lemma 1.

If (a) $\psi_\tau = a^2\psi_{\xi\xi} + h(\tau,\xi)$,

(b) $\psi(0,\xi)$ and $h(\tau,\xi)$ are C^∞ and P-periodic in ξ,

(c) there exist constants b, $0 < b < (\frac{2a\pi}{P})^2$, and c_n such that $\left|\frac{\partial^n h}{\partial\xi^n}(\tau,\xi)\right| \le c_n\, h(\tau,\xi)$ for $n \ge 0$, then there exist constants d_n, $n \geq 0$, such that

$$\text{(d)} \quad \left| \psi(\tau,\xi) - \frac{1}{P}\int_0^P \psi(0,\xi)d\xi - \frac{1}{P}\int_0^P\int_0^\infty h(\tau,\xi)d\tau\, d\xi \right| \leq d_o \exp(-b\tau)$$

$$\text{(e)} \quad \text{for } n \geq 1, \quad \left| \frac{\partial^n\psi}{\partial\xi^n}(\tau,\xi) \right| \leq d_n \exp(-b\tau).$$

Proof: Setting

$$\psi(\tau,\xi) = \sum_{-\infty}^{+\infty} A_n(\tau) \exp\left(+ \frac{2\pi in}{P}\xi\right),$$

$$h(\tau,\xi) = \sum_{-\infty}^{+\infty} \cdot B_n(\tau) \exp\left(+ \frac{2\pi in}{P}\xi\right),$$

the exact solution for the $A_n(\tau)$ is

$$A_n(\tau) = \exp\left(-\left(\frac{2\pi na}{p}\right)^2 \tau\right) \left[A_n(0) + \int_0^\tau \exp\left(+\left(\frac{2n\pi a}{P}\right)^2 s\right) B(s)ds\right]$$

where $A_n(0)$ is determined by the Fourier expansion of $\psi(0,\xi)$.

For n = 0, notice

$$A_0(\tau) = \frac{1}{P}\int_0^P \psi(0,\xi)d\xi + \frac{1}{P}\int_0^P\int_0^\tau h(s,\xi)ds ,$$

and since $h(\tau,\xi)$ decays exponentially in τ, $A_0(\tau) \to A_0(+\infty)$ constant as $\tau \to +\infty$.

In fact,

$$\left| A_0(\tau) - A_0(+\infty) \right| \le \left| \frac{1}{P}\int_0^P\int_\tau^\infty f(s,\xi)dsd\xi \right| \le \frac{c_o}{b}\exp(-b\tau).$$

For $n \neq 0$, using $|h(\tau,\xi)| \le c_o \exp(-b\tau)$ gives

$$|A_n(\tau)| \le \left[|A_n(0)| + \frac{c_o}{\left(\frac{2n\pi a}{P}\right)^2 - b} \right] \exp(-b\tau).$$

Combining the results for n=0 and $n\neq 0$ gives

$$|\psi(\tau,\xi) - A_0(+\infty)| \le \frac{c_o}{b} \exp(-b\tau)$$

$$+ \sum_{\substack{-\infty \\ n\neq 0}}^{+\infty} \left[|A_n(0)| + \frac{c_o}{\left(\frac{2n\pi a}{P}\right)^2 - b} \right] \exp(-b\tau)$$

and inequality (d) follows with

$$d_o = \frac{c_o}{b} + \sum_{\substack{-\infty \\ n \neq 0}}^{+\infty} \left(|A_n(0)| + \frac{c_o}{\left(\frac{2n\pi a}{P}\right)^2 -} \right)$$

(convergence of the $|A_n(0)|$ follows from smoothness of $\psi(0,\xi)$). To obtain (e) for the higher derivatives, apply (d) to the equation

$$\left(\frac{\partial^N \psi}{\partial \xi^N}\right)_\tau = a^2 \left(\frac{\partial^N \psi}{\partial \xi^N}\right)_{\xi\xi} + \frac{\partial^N h}{\partial \xi^N} \ .$$

The same arguments go through with

$A_n(\tau)$ replaced by $\left(\frac{2\pi i n}{P}\right)^N A_n(\tau)$,

$B_n(\tau)$ replaced by $\left(\frac{2\pi i n}{P}\right)^N B_n(\tau)$,

c_0 repaced by c_N ,

$$\int_0^P \frac{\partial^N \psi}{\partial \xi^N} d\xi + \int_0^P \int_0^\tau \frac{\partial^N h}{\partial \xi^N} ds d\xi = 0 \text{ by periodicity.}$$

Then (e) follows with

$$d_N = \frac{c_N}{b} + \sum_{\substack{-\infty \\ n \neq 0}}^{+\infty} \left(\frac{2n\pi}{P}^N |A_n(0)| + \frac{c_N}{\left(\frac{2\pi na}{P}\right)^2 - b} \right). \qquad \text{QED.}$$

Lemma 1 is now applied to $\phi_0(\tau,\xi)$, that is, Lemma 1 is applied with $\psi = \psi_0$, $a^2 = 1 + \alpha h_1$, $h(\tau,\xi) \equiv 0$, where ψ_0 is related to ϕ_0 by (4.2). From Lemma 1.d it folows that

$$\psi_0(\tau,\xi) \rightarrow \frac{1}{P}\int_0^P \psi_0(0,\xi)d\xi = \overline{\psi}_0 \tag{3.3a}$$

exponentially fast. In fact, from the most slowly decaying mode of in the proof of Lemma 1, we know that

$\psi_0(\tau,\xi) - \overline{\psi}_0$ and all ξ-derivatives of ψ_0 decay to 0 at the rate of

$$O\left(\exp\left(-\left(\frac{2\pi a}{P}\right)^2\right)\right) \quad . \tag{3.3b}$$

Consequently, as $\tau \to +\infty$,

$$\phi_0(\tau,\xi) \rightarrow \phi_0(+\infty) = \frac{1+\alpha h_1}{\ell_1+\alpha m_1} \; \ln\left[\frac{1}{P}\int_0^P \exp\left(\frac{\ell_1+\alpha m_1}{1+\alpha h_1}\,\phi_0(0,\xi)\right)d\xi\right] \; ,$$

all ξ-derivatives of $\phi_0 \rightarrow 0$, and the decay rate in both cases is (3.3c)

$$O\left(\exp\left(-(1+\alpha h_1)\left(\frac{2\pi}{P}\right)^2 \epsilon\, t\right)\right) .$$

To obtain a similar result for $\phi_n(\tau,\xi)$, notice that $h_n(\tau,\xi)$ in (3.2) is, by (2.2c.2), a polynomial in ξ-derivatives of $\phi_0(\tau,\xi)$, ..., $\phi_{n-1}(\tau,\xi)$ and functions of $\phi_0(0,\xi)$ such that $h_n \to 0$ if the ξ-derivatives of ϕ_0, ..., $\phi_{n-1} \to 0$. Consequently, if the ξ-derivatives of ϕ_0, ..., ϕ_{n-1} individually decay like $\exp(-b\tau)$ for $0 < b < \left(\frac{2\pi a}{p}\right)^2$, then so does $h_n(\tau,\xi)$ and all its ξ-derivatives (in particular, $h_1(\tau,\xi)$ is certainly bounded by $c\exp(-b\tau)$ for any b, $0 < b < \left(\frac{2\pi a}{p}\right)^2$, by the decay rate given in (3.3c)). The decay rate of the ξ-derivatives of ϕ_0, ..., ϕ_{n-1} can be assumed by induction, so the hypotheses of Lemma 1 are satisified. It follows that, as $\tau \to +\infty$,

$$\phi_n(\tau,\xi) \to \text{constant}, \tag{3.4}$$

all ξ-derivatives of $\phi_n \to 0$,

and the decay rate in both cases is faster than

$$O\left(\exp(-(1+\delta)(1+\alpha h_1)\left(\frac{2\pi}{p}\right)^2 \epsilon t)\right), \quad \text{where } \delta > 0.$$

To determine the behavior of u_1, v_1, it is necessary to know something about $B_1(\tau,\xi)$. Assuming $1-\alpha h_1 > 0$, we show that B_1 has a bounded

L_2-norm as $\tau \to +\infty$. It is sufficient to consider $\hat{B} = B_1(\tau,\xi) + f(\tau,\xi)$, since $f(\tau,\xi)$ consists of ξ-derivatives of ϕ_o' and decays exponentially in τ to 0. Equation (2.2c.3) for $\hat{B}$ can be written as ($b^2 = 1-\alpha h_1$)

$$\hat{B}_\tau = b^2\,[\hat{B}_{\xi\xi} + g_\xi\,\hat{B}_\xi] + g_1(\tau,\xi)\,\hat{B}, \tag{3.5a}$$

where g, g_1 are combinations of ξ-derivatives of ϕ_o', that is, they are P-periodic functions of ξ and decay exponentially in τ to 0. Equation (3.5a) can be simplified by a change of variables:

$$C(\tau,\xi) = \exp(g)\hat{B},$$

$$K(\tau,\xi) = g_{,\tau} - b^2(g_{\xi\xi} + g_\xi^2) + g_1, \tag{3.5b}$$

$$C_\tau = b^2 C_{\xi\xi} + K(\tau,\xi)\,C,$$

so $K(\tau,\xi)$ is P-periodic in ξ and decays exponentially fast in τ to 0. From (3.5b) follows

$$\frac{1}{2}\int_0^P (C^2)_\tau\, d\xi = -\,b^2\int_0^P C_\xi^2\, d\xi + \int_0^P K(\tau,\xi)C^2\, d\xi.$$

Using $|K(\tau,\xi)| \le \frac{k}{2}\exp(-d\tau)$ for some k, $d > 0$, we have

$$\left(\int_0^P C^2\, d\xi\right)_{,\tau} \le k\,\exp(-d\tau)\int_0^P C^2 d\xi\ .$$

Gronwall's inequality can now be applied (the following form is sufficient; see Coddington and Levinson (Chapter 1, 1955)).

Lemma 2. (Gronwall)

If $u(t)$, $v(t)$, $C \geq 0$ and $u(t) \leq C + \int_{t_o}^{t} v(s)u(s)ds$,

then $u(t) \leq C \exp\left(\int_{t_o}^{t} v(s)ds\right)$.

Equation (3.5e) now gives

$$\int_0^P C^2 d\xi \leq \left[\int_0^P C^2(0,\xi)d\xi\right] \exp\left(\frac{k}{d}(1 - \exp(-d\tau))\right), \qquad (3.5d)$$

so $\hat{B}(\tau,\xi)$ is bounded in the L^2-norm.

To derive the predictions, we first list expected behavior. From the results (3.3c) and (3.4) on the long time behavior of the individual terms ϕ_n, it seems reasonable to expect

$$\theta \sim t + \hat{\phi}, \quad \hat{\phi} = \phi_0(+\infty) + \epsilon\phi_1(+\infty) + \ldots, \qquad (3.6a)$$

as $t \to +\infty$, and that

$$\theta - t \text{ decays to } \hat{\phi} \text{ at a rate } O[\exp(-(1+ah_1)(\tfrac{2\pi}{P})^2 \epsilon t)]. \qquad (3.6b)$$

The initial conditions in (2.3) for $\phi_n(0,\xi)$, $n \geq 0$, are certainly independent of $B_1(0,\xi)$. Also, the equation for ϕ_0 is obviously independent of B_1, so we expect $\hat{\phi}$ to be independent of the initial conditions for $B_1(0,\xi)$, at least through $O(\epsilon)$. (In fact, the obtaining of equations (2.2c.1) for ϕ_n, $n \geq 1$, shows these equations depend only on the terms which are T-periodic in θ, and these terms are all independent of $B_n(\tau,\xi)$ for all $n \geq 1$, so every ϕ_n is independent of every B_m.) Since $B_1(\tau,\xi)$ remains bounded in the L_2-norm, it certainly seems reasonable to expect

$$B_1(\tau,\xi)\ \exp(-\mu\theta) \to 0 \tag{3.6c}$$

as $t \to +\infty$ for small ϵ, and the decay rate should be about $\exp(-\mu t)$.

Therefore, using (2.2c) for the structure of u_1, v_1, we expect the P_{10}, Q_{10} portion, consisting of T-periodic functions of θ and ξ-derivatives of ϕ_0, to decay to 0 at a rate like $O\left(\exp\left(-(1+\alpha h_1)\left(\frac{2\pi}{P}\right)^2 \epsilon t\right)\right)$, and the $\exp(-\mu\theta)$ portion to decay to 0 like $O(\exp(-\mu t))$; that is, we expect

$$u_1 v_1 \to 0 \text{ at a rate } O[\exp(-(1+\alpha h_1)(2\pi/P)^2 \epsilon t)]. \tag{3.6d}$$

Prediction I now follows directly from applying (3.6a) and (3.6d) to (3.1) and adding the expected independence of $\hat{\phi}$ from $B_1(0,\xi)$.

Prediction II follows from the decay rates in (3.6b), (3.6d).

The first half of Prediction III follows from (3.6a) together with the expresion for $\phi_0(+\infty)$ in (3.3c). The second half of Prediction III, for initial data of the form $\phi_0(0,\xi) = A\sin(\frac{2k\pi}{P}\xi)$ follows from Lemma 3, a generalization of Bessel's integral representation for Bessel functions.

Lemma 3.

(a) Set $y(A) = \frac{1}{P}\int_0^P f\left(A\sin(\frac{2\pi k}{P}\xi)\right)d\xi$, $k = 1,2, \ldots$

If $f(x)$ is a smooth function satisfying $f''(x) - \alpha x f'(x) - \beta f(x) = 0$, then $y(A)$ is smooth, $y(0) = f(0)$, and

$$\frac{d^2y}{dA^2} + \frac{1-\alpha A}{A}\frac{dy}{dA} - \beta y = 0.$$

(b) $\frac{1}{P}\int_0^P \exp\left(A\sin(\frac{2\pi k}{P}\xi)\right)d\xi = I_o(A).$

Proof: Simplify by

$$y(A) = \frac{1}{P}\int_0^P f\left(A\sin(\frac{2\pi k}{P}\xi)\right)d\xi = \int_0^1 f(A\sin 2\pi k\xi)d\xi ,$$

so only the latter integral need be considered. If f is continuous, obviously $f(0) = y(0)$. Now notice

$$\frac{d^2y}{dA^2} = \int_0^1 f''(A \sin 2\pi k\xi)\,d\xi$$

$$-\int_0^1 \frac{\cos(2\pi k\xi)}{2\pi kA}\; f''(A \sin 2\pi k\xi)\; 2\pi kA \cos(2\pi k\xi)\; d\xi$$

$$= \int_0^1 f''(A \sin 2\pi k\xi)\,d\xi - \frac{1}{A}\int_0^1 f'(A \sin 2\pi k\xi) \sin 2\pi k\xi\, d\xi$$

$$= \alpha A \frac{dy}{dA} + \beta y - \frac{1}{A}\frac{dy}{dA}\,.$$

For (b), pick $\alpha = 0$, $\beta = 1$, $f(x) = \exp(x)$, and the equation for y is a modified Bessel equation. The initial condition $y(0) = \exp(0)$ gives $y(A) = I_o(A)$. QED

CHAPTER V

NUMERICAL SOLUTIONS OF REACTION-DIFFUSION EQUATIONS

Introduction

This chapter is concerned with the numerical solutions of two-component reaction-diffusion systems of the form

$$u_t = F(u,v) + (1+\alpha)\,\epsilon\, u_{\xi\xi}$$

$$v_t = G(u,v) + (1-\alpha)\,\epsilon\, v_{\xi\xi}\,, \quad |\alpha| \leq 1, \tag{1.1a}$$

with initial data periodic in ξ with period $P = 1$.

The chapter contains two separate topics. The first topic (Sections 2, 3, 4) concerns the numerical check of the predictions made in Chapter IV on the behavior of solutions of reaction-diffusion equations. The second topic (Sections 5, 6, 7) concerns the numerical stability of finite difference schemes for nonlinear diffusion equations.

Lees' method was used for the numerical work of Sections 2, 3, 4. Section 2 gives a brief discussion of this finite difference scheme and a detailed discussion of numerical problems in validating Predictions I-III of Chapter IV.

Section 3 checks the predictions for a λ-ω system; Section 4 for a case of the solvable chemical reactor system mentioned in Chapter III. It is necessary to write the initial data in the form used in Chapter IV:

$$\begin{bmatrix} u(0,\xi) \\ v(0,\xi) \end{bmatrix} = \begin{bmatrix} U(\phi_o(0,\xi)) \\ V(\phi_o(0,\xi)) \end{bmatrix} \tag{1.1b}$$

$$+ \epsilon B_I(0,\xi) \exp(-\mu\phi_o(0,\xi)) \begin{bmatrix} \hat{U}(\phi_o(0,\xi)) \\ \hat{V}(\phi_o(0,\xi)) \end{bmatrix} ,$$

where (U, V) is the T-periodic limit cycle solution of the kinetic systems and $-\mu$, $\hat{U}$, $\hat{V}$ are related to solutions of the variational equation about the *limit cycle (see Lemma C)*. The three predictions to be checked concern the evolution of solutions to $U(t + \hat{\phi})$, $V(t + \hat{\phi})$, the rate at which the evolution takes place, and the dependence of $\hat{\phi}$ on the initial data. To test these, it is necessary to know certain functions (U, V, U', V', $\hat{U}$, $\hat{V}$) and certain constants, such as the Floquet exponent $-\mu$ and

$$h_1 = \frac{1}{T}\int_0^T \frac{U'\hat{V} + V'\hat{U}}{U'\hat{V} - V'\hat{U}}\,dt \ , \quad \ell_1 = \frac{1}{T}\int_0^T \frac{U''\hat{V} - V''\hat{U}}{U'\hat{V} - V'\hat{U}}\,dt, \tag{1.2}$$

$$m_1 = \frac{1}{T}\int_0^T \frac{U''\hat{V} + V''\hat{U}}{U'\hat{V} - V'\hat{U}}\,dt.$$

Sections 3 and 4 calculate these quantities for their respective systems and proceed with the numerical checks. Briefly, all three predictions hold for the λ-ω system of Section 3; the first two clearly hold for the chemical reactor system of Section 4 and the third prediction appears hold. In this last case, however, only indirect evidence is available: the results of the third prediction appear to hold when the numerical results for small ϵ are extrapolated to very small ϵ, but it is not numerically feasible to directly check the cases with those very small values.

The remainder of the chapter is concerned with numerical questions only.

Information on numerical methods for diffusion equations is somewhat scattered. As general references, Carnahan, Luther, and Wilkes (1969) and Carrier and Pearson (1976) should be mentioned--Carrier and Pearson give a particularly excellent discussion of numerical stability. More specific references are Rinzel (1977, especially concerned with calculating traveling fronts), Varah (1978, concerned with numerical stability), and Fornberg (1973, which gives some discussion of numerical stability in nonlinear cases). Lees' Method originally appeared in Lees (1969).

Section 4 gives a brief survey of finite difference methods for solving diffusion equations: the explicit, Crank-Nicolson, Lees', and modified Lees' methods. The concept of numerical stability is defined, and the stability properties of the methods are derived for linear equations with constant coefficients. The programming of Lees' method for periodic initial data is also discussed.

Numerical stability of a finite difference scheme is usually determined by how the method works for a PDE with constant coefficients. For such simple PDEs the finite difference solution can usually be found explicitly and the boundedness of solutions determined directly.

However, very little is known about the stability of difference schemes applied to nonlinear systems, and Sections 5 and 6 are concerned with nonlinear numerical stability.

My interest in this problem originated in a seminar on finite difference methods for PDEs given by Dr. James Varah of the University of British Columbia. It seemed that the geometric arguments of Chueh, Conley, and Smoller (1977, discussed in Chapter I) would carry over to the discrete equations and provide stability results for finite difference methods applied to nonlinear diffusion systems. This work is carried out in Section 6. The proofs suggest an essential difference between numerical stability for linear and nonlinear cases: for linear problems, stability is usually a matter of wavelength alone, but in nonlinear problems both wavelength and amplitude may be involved. An example is given at the end of Section 6; it gives an explicit finite difference solution to a nonlinear, scalar diffusion equation (whose continuous soutions all decay to 0 as $t \to +\infty$). The explicit solution also goes to 0 if the initial amplitude is small but blows up if the amplitude is $O(1/\sqrt{\Delta t})$.

The geometric proofs only yield a conditional stability requirement $\Delta t = O(\Delta x^2)$ for all methods in Section 5; since some of these are unconditionally stable for linear systems, stronger results appeared possible. Section 7 obtains direct estimates which show that the Lees' and modified Lees' methods are unconditionally stable. (Incidentally, Lemma 1, a key step in the proof, is of interest in its own right.)

Numerical Procedures

The numerical problems occurring in calculating the predicted asymptotic phase $\hat{\phi}$ are rather awkward. First, the decay rate to a spatially homogeneous solution is $\exp(-C\epsilon t)$, where C is some constant and ϵ is small. Consequently, it is not economically possible to obtain the asymptotic phase $\hat{\phi}$ for exceptionally small ϵ --to validate the predictions of Chapter IV it must be possible to choose ϵ small, but at the same time it must be sufficiently large that decay to a spatially homogeneous solution takes place in a computable amount of time. Second, in spite of the long period of time necessary for a spatially homogeneous solution $U(t+\hat{\phi})$, $V(t+\hat{\phi})$ to form, the numerically obtained asymptotic phase (called ϕ_{obs} here) must yield an accurate value for $\hat{\phi}$ in order to check Prediction III. This section discusses how these problems were solved in practice.

Section 5 discusses three numerical algorithms for diffusion equations: the explicit method, the Crank-Nicolson method, and Lees' method. The explicit method requires $\Delta t = O(\Delta x^2)$ as a numerical stability restriction, which makes it very expensive for integration over long time periods. The Crank-Nicolson method is numerically stable but requires the solution of a large system of nonlinear equations for each time step when applied to a nonlinear diffusion system (as here). Lees' method is an extrapolated version of Crank-Nicolson using 3 time levels. It has the same accuracy and stability as Crank-Nicolson but only requires the solution of a large linear system at each time step, even if the diffusion system is nonlinear. Lees' method was used in the calculations and worked quite well.

In connection with the difficulty of choosing ϵ small but not so small that the decay rate is impracticably slow, another difficulty, which limited ϵ-values to $\epsilon < .01$, should be mentioned. All initial data were taken on $0 \leq \xi \leq 1$ with periodic initial conditions; the standard step size was $\Delta\xi = .02$ (except for certain accuracy checks with $\Delta\xi = .01$). This step size and boundary conditions meant a 50x50 linear system had to be solved at each time step (fortunately, it was nearly tridiagonal). Values of ϵ larger than about .01 led to "exponential underflow" error messages during the inversion; however, no attempt was made to root out the difficulty since only small values of ϵ were relevant in the calculations.

Fortunately, for the examples studied in Sections 3 and 4, $\epsilon \sim .01$ gave decay rates resulting in spatially homogeneous solutions by $t \sim 8\pi$, and this time interval (together with the relatively large time steps made possible by the procedure discussed next) was economically feasible. Cutting ϵ by a factor of 10 would require a time interval 10 times longer for the solution to decay to a spatially homogeneous solution, so no runs with $\epsilon = .001$ (and a necessary time interval 80π) were made.

The most serious problem was the accumulated numerical error in ϕ_{obs}, the numerically calculated asymptotic phase. For instance, one of the larger phase shifts predicted was .12, and this shift had to be accurately measured over a time interval of $8\pi \sim 26$. In principle, once the time interval required was known to be 8π, so integration takes place over the rectangle $0 \leq \xi \leq 1$, $0 \leq t \leq 8\pi$, the accuracy could be improved by decreasing $\Delta\xi, \Delta t$. In practice, of course, sufficiently small step sizes were not economically possible-- the high cost limited their use to occasional checks of accuracy.

However, the following idea retains accuracy while permitting relatively large time steps. Since we are concerned with solutions which perturb the limit cycle solution, the numerical error involved should be nearly the same as the numerical error for the limit cycle alone. (This is not necessarily the case if abrupt spatial changes occur, but here only mild spatial changes occur.) When Lees' method is applied to the limit cycle alone, the spatial terms cancel out and the method reduces to a discrete method for solving a system of ODE's; calculations can then be carried out on a programmable pocket calculator.

For ex::nle, consider a reaction-diffusion system with kinetic equations (this system is the example used in Section 3)

$$\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 1-R^2 & -\frac{1}{2}(1+R^2) \\ \frac{1}{2}(1+R^2) & 1-R^2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}, \quad u=R\cos\psi, \quad v=R\sin\psi, \qquad (2.1a)$$

with limit cycle solution

$$\begin{bmatrix} U(t) \\ V(t) \end{bmatrix} = \begin{bmatrix} \cos t \\ \sin t \end{bmatrix}, \text{ period } T = 2\pi. \qquad (2.1b)$$

Table 4A shows the results obtained when we begin at the point $(u_0,v_0) = (1,0)$ on the limit cycle and integrate using step sizes $\Delta t = 2\pi/100$ and $\Delta t = 2\pi/600$. In both cases the error in R^2 is negligible. The error in ϕ is negligible for $\Delta t = 2\pi/600$; however for $\Delta t = 2\pi/100$ it is large enough to affect calculations of the asymptotic phase ϕ. The phase error in solving the kinetic equations will be called the Kinetic Phase Error (KPE).

Table 4B gives results for the reaction-diffusion system with kinetic equations (used as an example in Section 4)

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} (1-u^2)\,u - v \\ u + (1-u^2)v \end{bmatrix} \tag{2.2a}$$

with limit cycle

$$\begin{bmatrix} U(t) \\ V(t) \end{bmatrix} = \begin{bmatrix} R_o(t)\cos t \\ R_o(t)\sin t \end{bmatrix}, \tag{2.2b}$$

$$R_o(t) = \left(\frac{2(1+a^2)}{1+a^2 + a^2\cos 2t + a\sin 2t}\right)^{1/2}, \quad \text{period } T = 2\pi.$$

The KPE can be used to improve accuracy in the following way: let initial data be given for either (2.1) or (2.2) and compute the solutions up to $t = 2n\pi$, at which point they are found to be spatially homogeneous with the form

TABLE 4A

Kinetic Phase Error (KPE) for (2.1)

	time steps	R^2 exact	R^2 calc.	exact	calc. (= $2n\pi$ + KPE)
$\Delta t = 2\pi/100$	0	1.00	--	0	--
	100	1.00	.99710	2π	2 + .01215
	200	1.00	.99710	4π	4 + .02271
	300	1.00	.99710	6π	6 + .03326
	400	1.00	.99710	8π	8 + .04382
	800	1.00	.99710	16π	16 + .08605
$\Delta t = 2\pi/600$	0	1.00	--	0	--
	600	1.00	.99992	2π	2 + .00034
	1,200	1.00	.99992	4π	4 + .00062
	1,800	1.00	.99992	6π	6 + .00091
	2,400	1.00	.99992	8π	8 + .00112

TABLE 4B

Kinetic Phase Error (KPE) for (2.2)

	time steps	exact	calc. (= $2n\pi$ + KPE)
$\Delta t = 2\pi/100$	0	0	--
	100	2π	2 - .00115
	200	4π	4 - .00359
	300	6π	6 - .00602
	400	8π	8 - .00846
	600	12π	12 - .01333
	800	16π	16 - .01820
	1,600	32π	32 - .03767

$$\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} U(2n\pi + \phi_{obs}) \\ V(2n\pi + \phi_{obs}) \end{bmatrix} .$$

Then the calculated asymptotic phase is $\phi_{obs} = \hat{\phi}$ + error. We expect this (phase) error for the perturbed limit cycle solution and the KPE for the limit cycle solution alone to be about the same, since the solutions are nearly equal and the same finite difference method is applied in each case. Consequently, ϕ_{num}, defined by

$$\phi_{num} \equiv \phi_{obs} - \text{KPE} \tag{2.3}$$

should give a more accurate estimate of ϕ. This is, in fact, the case--Section 3 and 4 both compare ϕ_{num} obtained for $\Delta t = 2\pi/100$ against ϕ_{obs} for $\Delta t = 2\pi/600$ and the agreement is excellent. This procedure allows us to make standard use of the relatively large time steps $\Delta t = 2\pi/100$.

As a specific example, consider a calculation actually carried out in obtaining results at the beginning of Section 3. The reaction-diffusion system is

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} 1-R^2 & -\frac{1}{2}(1+R^2) \\ \frac{1}{2}(1+R^2) & 1-R^2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} (1+\alpha)\epsilon u_{\xi\xi} \\ (1-\alpha)\epsilon v_{\xi\xi} \end{bmatrix} .$$

A solution is found using $\Delta t = 2\pi/100$ with initial data

$$\begin{bmatrix} u(0,\xi) \\ v(0,\xi) \end{bmatrix} = \begin{bmatrix} \cos(\sin(2\pi\xi)) \\ \sin(\sin(2\pi\xi)) \end{bmatrix} .$$

At $t = 8\pi$, the solution is found to be essentially spatially homogeneous and is found to have the form

$$\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \cos(8\pi - .085) \\ \sin(8\pi - .085) \end{bmatrix} .$$

Then $\phi_{obs} = -.085$ and the improved estimate of $\hat{\phi}$ is $\phi_{num} = \phi_{obs} - KPE$ $= -.085 -(.044) = -.129$. (When the solution was rerun using the much smaller time steps $\Delta t = 2\pi/600$, then $\phi_{obs} = -.129$ actually occurred!)

Check of Predictions: λ-ω Systems

Relevant information on λ-ω systems, in general, is summarized first (from Chapter III, equations (2.5ff)). Then the specific system studied numerically is given, and the three predictions are worked out in detail and compared with the numerical results.

By definition, a λ-ω system has the form (1.1a) with $(u = R\cos\psi,\ v = R\sin\psi)$

$$\begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} = \begin{bmatrix} \lambda(R) & -\lambda(R) \\ \omega(R) & \omega(R) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \tag{3.1a}$$

and a stable limit cycle

$$\begin{bmatrix} U(t) \\ V(t) \end{bmatrix} = \begin{bmatrix} R_o \cos(\omega_o t) \\ R_o \sin(\omega_o t) \end{bmatrix} ,$$

$$\lambda(R_o) = 0, \ \lambda'(R_o) < 0, \ \omega_o = \omega(R_o), \ T = \frac{2\pi}{\omega_o} . \tag{3.1b}$$

The fundamental matrix of the variational equation about the limit cycle is

$$\begin{matrix} U'(t) & \exp(-\mu t)\,\hat{U}(t) \\ V'(t) & \exp(-\mu t)\,\hat{V}(t) \end{matrix} =$$

$$\begin{matrix} -R_o \omega_o \sin(\omega_o t) & -\dfrac{\exp(-\mu t)}{R_o \omega_o \cos \sigma_o} \cos(\omega_o t + \sigma_o) \\ R_o \omega_o \cos(\omega_o t) & -\dfrac{\exp(-\mu t)}{R_o \omega_o \cos \sigma_o} \sin(\omega_o t + \sigma_o) \end{matrix} , \tag{3.1c}$$

$-\mu = R_o \lambda'(R_o)$, with $S_o \cos \sigma_o = \lambda'(R_o)$, $S_o \sin \sigma_o = \lambda'(R_o)$.

Using (1.2), the basic constants become

$$h_1 = 0, \ \ell_1 = \frac{\omega_o \, \omega'(R_o)}{\lambda'(R_o)} , \ m_1 = 0. \tag{3.1d}$$

The specific λ-ω system used in the numerical calculations is

$$\begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} = \begin{bmatrix} 1 - R^2 & -\frac{1}{2}(1+R^2) \\ \frac{1}{2}(1+R^2) & 1 - R^2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \tag{3.2a}$$

with stable limit cycle

$$\begin{bmatrix} U(t) \\ V(t) \end{bmatrix} = \begin{bmatrix} \cos t \\ \sin t \end{bmatrix}, \quad R_o = 1, \quad \omega_o = 1, \quad T = 2\pi. \tag{3.2b}$$

The fundamental matrix of the variational equation about the limit cycle is

$$\begin{bmatrix} U'(t) & \exp(-\mu t)\,\hat{U}(t) \\ V'(t) & \exp(-\mu t)\,\hat{V}(t) \end{bmatrix} \tag{3.2c}$$

$$\begin{bmatrix} -\sin t & -\dfrac{\exp(-2t)}{\cos \sigma_o} \cos(t+\sigma_o) \\ \cos t & -\dfrac{\exp(-2t)}{\cos \sigma_o} \sin(t+\sigma_o) \end{bmatrix}, \quad \begin{matrix} \cos \sigma_o = -2/\sqrt{5}, \\ \sigma_o = 2.6774 \text{ rad.} \end{matrix}$$

The basic constants are

$$h_1 = 0, \; \ell_1 = -\frac{1}{2}, \; m_1 = 0. \tag{3.2d}$$

We are now ready to being checking the three predictions of Section 4, Chapter IV.

Check I. The period in ξ is taken to be $P = 1$. Initial data are

$$\begin{bmatrix} u(0,\xi) \\ v(0,\xi) \end{bmatrix} = \begin{bmatrix} \cos(\sin(2\pi\xi)) \\ \sin(\sin(2\pi\xi)) \end{bmatrix} \tag{3.3}$$

$$+ \epsilon \tilde{B}(0,\xi) \begin{bmatrix} \cos(\sin(2\pi\xi) + 2.677945) \\ \sin(\sin(2\pi\xi) + 2.677945) \end{bmatrix},$$

that is, $\phi_o(0,\xi) = \sin(2\pi\xi)$

$$B_1(0,\xi) = \frac{2}{\sqrt{5}} \exp(+ 2 \sin(2\pi\xi)) \; \tilde{B}(0,\xi).$$

Prediction I says the solution should evolve to a spatially homogeneous solution $(U(t+\hat{\phi}), V(t+\hat{\phi}))$ and that $\hat{\phi}$ is independent of $B_1(0,\xi)$, that is, of $\tilde{B}(0,\xi)$. This prediction was checked by using several pairs of values ϵ, q and for each pair solutions for $\epsilon\tilde{B}(0,\xi) \equiv 0$, $\equiv .1$ were carried to $t = 4T = 8\pi$. Each solution evolved to a spatially homogeneous one with amplitude $(u^2 + v^2) = 1$. The values of ϕ_{obs}, ϕ_{num} are given in Table 5A. Notice $\tilde{B}(0,\xi)$ in these runs are .1/.006= 16.7 and .1/.01 = 10. Clearly the asymptotic phase is independent of $\tilde{B}(0,\xi)$ for small $\tilde{B}(0,\xi)$. Runs were also made with $\epsilon\tilde{B}(0,\xi) \equiv .5$ (or $\tilde{B}(0,\xi) = 83.3, 50$), but in these cases the result differed from the case with $\tilde{B}(0,\xi) \equiv 0$, indicating the perturbation was too large.

TABLE 5A

Check of Prediction I for (3.2)
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, $\phi_{num} = \phi_{obs} - .044$, carried to $t = 8\pi$.

		$\epsilon\tilde{B}(0,\xi) \equiv .0$		$\epsilon\tilde{B}(0,\xi) \equiv .1$	
ϵ	α	ϕ_{obs}	ϕ_{num}	ϕ_{obs}	ϕ_{num}
.006	2/3	$-.123 \pm .003$*	$-.167 \pm .003$	$-.123 \pm .003$	$-.167 \pm .003$
.010	0	$-.085$	$-.129$	$-.083$	$-.127$
.006	$-2/3$	$-.075 \pm .003$	$-.119 \pm .003$	$-.072 \pm .003$	$-.116 \pm .003$

TABLE 5B

Check of Prediction I with small time steps for (3.2)
$\Delta\xi = .02$, $\Delta t = 2\pi/600$, $\phi_{num} = \phi_{obs} - .001$, carried to $t = 8\pi$.

		$\epsilon\tilde{B}(0,\xi) \equiv .0$		$\epsilon\tilde{B}(0,\xi) \equiv .1$	
ϵ	α	ϕ_{obs}	ϕ_{num}	ϕ_{obs}	ϕ_{num}
.006	2/3	$-.167 \pm .003$	$-.168 \pm .003$	$-.166 \pm .003$	$-.167 \pm .003$
.010	0	$-.129$	$-.130$	$-.127$	$-.128$
.006	$-2/3$	$-.119 \pm .003$	$-.120 \pm .003$	$-.115 \pm .003$	$-.116 + .003$

*The notation $-.123 \pm .003$ means the minimum and maximum values observed were $-.123 - .003$ and $-.123 + .003$, respectively.

This situation was also used to make a check of the accuracy of the ϕ_{num}-formula (2.3). Exactly the same runs as above were made, but with $\Delta t = 2\pi/600$ instead of $2\pi/100$. The results are shown in Table 5E. Since there is excellent agreement between ϕ_{num} in the $\Delta t = 2\pi/100$, $2\pi/600$ cases, we take the ϕ_{num}-formula (2.3) as a valid means of correction and in the remaining tables of data only ϕ_{num} will be given.

Check II. Prediction II deals with the rate of decay to a spatially homogeneous solution, so some measure of the perturbation amplitude is needed. Notice that solutions periodic in ξ become closed curves when sketched in the phase plane as a function of ξ with t fixed (Figure 5). As t increases, the curve shrinks to a (moving) point on the limit cycle because a function constant with respect to ξ is just a point. Therefore, a reasonable measure of amplitude for functions with period 1 in ξ is

$$A(t) = \max_{0\leq\xi\leq 1} \text{Arctan}\,(v/u) - \min_{0\leq\xi\leq 1} \text{Arctan}\,(v/u). \qquad (3.4)$$

Equation (3.3) with $\tilde{B}(0,\xi) \equiv 0$ is taken as initial data. The amplitude $A(t)$ is measured at regular intervals $t = 0, 2\pi, 4\pi, \ldots$. According to Prediction II, the decay rate should be $\exp(-4\pi^2 \epsilon t)$, that is, the ratio $A(2(n+1)\pi)/A(2n\pi) \sim \exp(-8\pi^3\epsilon)$. The results shown in Table 6 clearly confirm this prediction.

AD-A087 114 CENTER FOR NAVAL ANALYSES ALEXANDRIA VA OPERATIONS EV--ETC F/G 7/4

LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS.(U)

JUN 80 D COPE

UNCLASSIFIED OEG-PP-287 NL

3 OF 4

AD A
087114

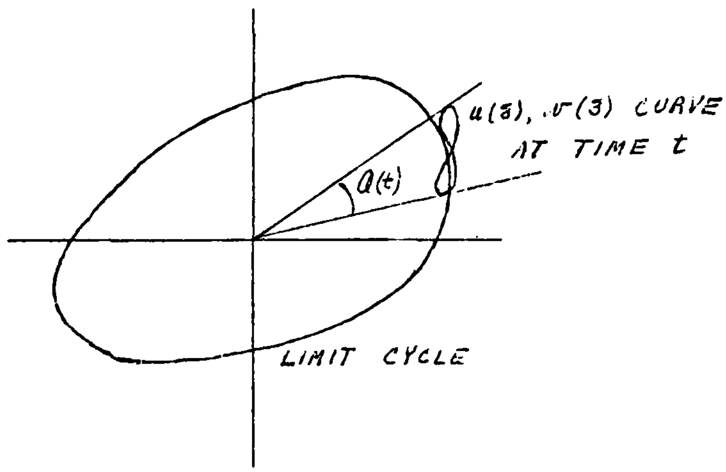


FIGURE 5. THE ANGULAR AMPLITUDE FUNCTION $a(t)$.

TABLE 6

Check of Prediction II (predicted ratio = $\exp(-8\pi^3\epsilon)$) for (3.2).
$\Delta\xi = .02$, $\Delta t = 2\ /100$

	$\epsilon = .006$, $\alpha = 2/3$ predicted ratio = .226		$\epsilon = .010$, $\alpha = .0$ predicted ratio = .084		$\epsilon = .006$, $\alpha = -2/3$ predicted ratio = .226	
t	A(t)	ratio	A(t)	ratio	A(t)	ratio
0	2.000	---	2.000	---	2.000	---
2π	.476	.24	.173	.09	.478	.24
4π	.110	.23	.014	.08	.112	.23
6π	.026	.24	.001	.07	.026	.24
8π	.006	.23	.000	---	.006	.23

<u>Check III</u>. For Prediction III, the initial data is taken as

$$\begin{bmatrix} u(0,\xi) \\ v(0,\xi) \end{bmatrix} = \begin{bmatrix} \cos(A \sin(2\pi\xi)) \\ \sin(A \sin(2\pi\xi)) \end{bmatrix} \tag{3.5}$$

$$\text{or } \phi_0(0,\xi) = A \sin(2\pi\xi), \quad B_1(0,\xi) \equiv 0,$$

and $A = .5$, 1.0 will be used. Prediction III then gives the values of $\hat{\phi}$ as (since $I_0(x)$ is an even function):

$$\hat{\phi} = -2 \ln \left(I_0\left(\tfrac{1}{2} A\right)\right) + O(\epsilon). \tag{3.6}$$

The results are shown in Tables 7A, B for $A = .5$, 1.0, respectively. For $A = .5$ the values are excellent. For $A = 1$, they are excellent for $\alpha \leq 0$ but begin to differ noticeably as $\alpha \rightarrow +1$.

Two possible reasons for the increased error as $\alpha \rightarrow +1$ are

(a) numerical error due to values of $\Delta\xi, \Delta t$ which are too large,

(b) or the $O(\epsilon)$-term is significant (that is, ϵ is not sufficiently small).

The first possibility is easily checked. The solution for $\epsilon = .0060$, $\alpha = 2/3$, $A = 1$ is calculated using smaller step sizes $\Delta\xi = .01$, $\Delta t = 2\pi/600$. At $t = 8\pi = 4T$, $\phi_{num} = -.167 \pm .003$ in exact agreement with Table 7B. The discrepancy as $\alpha \rightarrow +1$ is definitely not numerical error.

The second possibility is the size of ϵ. The simplest way to run a check is to reduce ϵ and see if the discrepancy reduces. The two worst cases ($\epsilon = .010$, $\alpha = 9/10$; $\epsilon = .006$, $\alpha = 2/3$) of Table 7B were rerun with the same $\Delta\xi, \Delta t$ values, but with ϵ cut in half: .005, .003. (It was necessary to run the solution twice as long to smooth it out.)

The results are shown in Table 7C. Cutting ϵ in half cut the discrepancy in half and therefore the discrepancy is clearly due to an $O(\epsilon)$ contribution.

The numerical solutions verify the predictions of Chapter IV of convergence to a spatially uniform solution, the rate of convergence, and the asymptotic phase resulting from that convergence.

Check of Predictions: the Solvable Chemical Reactor System

The calculations of the last section will be repeated for the system with kinetics

$$\begin{bmatrix} F(u,v) \\ G(u,v) \end{bmatrix} = \begin{bmatrix} a(1-u^2)u-v \\ 1+a(1-u^2)v \end{bmatrix} . \tag{4.1a}$$

This system, which arises in connection with chemical reactors, has already been studied in Chapter III. The limit cycle can be given explicitly as

$$\begin{bmatrix} U(t) \\ V(t) \end{bmatrix} = \begin{bmatrix} R_o(t) \cos t \\ R_o(t) \sin t \end{bmatrix} \tag{4.1b}$$

$$R_o(t) = \left(\frac{2(1 + a^2)}{1 + a^2 + a^2 \cos 2t + a \sin 2t} \right)^{1/2}, \quad T = 2\pi.$$

TABLE 7A

Check of Prediction III for (3.2); $\phi_o(0,\xi) = \frac{1}{2}\sin(2\pi\xi)$ $(A = \frac{1}{2})$
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, carried to $t = 8\pi$

ϵ	α	ϕ_{num}	$\phi_o(+\infty) = -2\ln(I_o(.25))$	discrepancy
.0060	2/3	$-.043 \pm .002$	$-.031$	.012
.0075	1/3	$-.037$	$-.031$	.006
.0100	0	$-.031$	$-.031$	.000
.0075	$-1/3$	$-.027$	$-.031$	.004
.0060	$-2/3$	$-.026 \pm .002$	$-.031$	.005

TABLE 7B

Check of Prediction III for (3.2); $\phi_o(0,\xi) = \sin(2\pi\xi)$ $(A = 1)$
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, carried to $t = 8\pi$

ϵ	α	ϕ_{num}	$\phi_o(+\infty) = -2\ln(I_o(.5))$	discrepancy
.0100	9/10	$-.225$	$-.123$	.102
.0060	2/3	$-.167 \pm .003$	$-.123$	.044
.0075	1/3	$-.147 \pm .001$	$-.123$	.024
.0100	0	$-.129$	$-.123$	.006
.0075	$-1/3$	$-.118 \pm .001$	$-.123$	.005
.0060	$-2/3$	$-.119 \pm .003$	$-.123$	.004
.0100	$-9/10$	.118	$-.123$	.005

TABLE 7C

Decrease in discrepancy when ϵ is decreased $(\phi_o(0,\xi) = \sin 2\pi\xi)$
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, carried to $t = 8\pi$

ϵ	α	ϕ_{num}	$\phi_o(+\infty) = -2\ln(I_o(.5))$	discrepancy
.005	9/10	$-.181$	$-.123$	.058
.003	2/3	$-.148 \pm .003$	$-.123$	.025

The fundamental matrix of the variational equation about the limit cycle is

$$\begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U}(t) \\ V'(t) & \exp(-\mu t)\hat{V}(t) \end{bmatrix} = \begin{bmatrix} R_o' \cos t - R_o \sin t & \exp(-2at)R_o^3 \cos t \\ R_o' \sin t + R_o \cos t & \exp(-2at)\, R_o^3 \sin t \end{bmatrix}, \tag{4.1b}$$

with Wronskian $= -\exp(-2at)R_o^4$.

Using (1.2), the constants are defined by integrals so:

$$h_1 = \frac{1}{2\pi}\int_o^{2\pi}\left(-\frac{R_o'}{R_o}\sin 2t - \cos 2t\right)dt,$$

$$\ell_1 = \frac{1}{2\pi}\int_o^{2\pi}\left(\frac{2R_o'}{R_o}\right)dt,$$

$$m_1 = \frac{1}{2\pi}\int_o^{2\pi}\left[\left(1 - \frac{R_o''}{R_o}\right)\sin 2t - \frac{2R_o'}{R_o}\cos 2t\right]dt.$$

Notice that integration by parts and periodicity of R_0 gives

$$\int_o^{2\pi}\frac{-R_o''}{R_o}\sin 2t\, dt = \int_o^{2\pi} R_o'\left(\frac{2\cos 2t}{R_o} - \frac{R_o'\sin 2t}{R_o^2}\right)dt.$$

The integrals simplify to

$$h_1 = -\frac{1}{2\pi}\int_o^{2\pi} \frac{R_o'}{R_o} \sin 2t \ dt,$$

$$\ell_1 = 0$$

$$m_1 = -\frac{1}{2\pi}\int_o^{2\pi} \left(\frac{R_o'}{R_o}\right)^2 \sin 2t \ dt.$$

The evaluation of the first can be done as follows:

$$\text{set } I_1 = \int_o^{2\pi} \frac{R_o'}{R_o} \sin 2t \ dt$$

$$= \int_o^{2\pi} \frac{a^2 \sin 2t - a \cos 2t}{1 + a^2 + a^2 \cos 2t + a \sin 2t} \sin 2t \ dt$$

$$= \int_o^{2\pi} \frac{a^2 \sin t - a \cos t}{1 + a^2 + a^2 \cos t + a \sin t} \sin t \ dt$$

$$= \int_o^{2\pi} \frac{\sin (t - A) \sin t}{b + \cos (t - A)} dt, \quad \text{where } \cos A = \frac{a}{\sqrt{a^2+1}},$$

$$\sin A = \frac{a}{\sqrt{a^2+1}},$$

$$b = \frac{1}{a}\sqrt{a^2+1} > 1 \text{ for } a > 0,$$

$$= \int_o^{2\pi} \frac{\sin t \ \sin (t + A)}{b + \cos t} \, dt \quad \text{by periodicity in } t,$$

$$= (\cos A) \int_o^{2\pi} \frac{(\sin t)^2}{b + \cos t} \, dt, \quad \text{since the odd parts of the integrand integrate to 0,}$$

$$= (\cos A) \int_o^{2\pi} \frac{1 - [(b + \cos t) - b]^2}{b + \cos t} \, dt$$

$$= (\cos A) \left[2\pi b + (1 - b^2) \int_o^{2\pi} \frac{dt}{b + \cos t} \right] .$$

The last integral can be evaluated by the Residue Theorem,

$$\int_o^{2\pi} \frac{dt}{b + \cos t} = \frac{2}{\sqrt{b^2 - 1}} \quad , \quad b > 1,$$

so $I_1 = 2\pi(\cos A) \left(b - \sqrt{b^2 - 1} \right)$.

Similarly, set

$$I_2 = \int_o^{2\pi} \left(\frac{R_o'}{R_o}\right)^2 \sin 2t \, dt$$

$$= \int_o^{2\pi} \left(\frac{a^2 \sin 2t - a \cos 2t}{1 + a^2 + a^2 \cos 2t + a \sin 2t}\right)^2 \sin 2t \, dt$$

$$= (\sin A) \int_0^{2\pi} \frac{(\sin t)^2 \cos t}{(b + \cos t)^2} dt \quad \text{with b, A as above,}$$

$$= (\sin A) \left[\int_o^{2\pi} \frac{(\sin t)^2}{b + \cos t} dt - b \int_o^{2\pi} \frac{(\sin t)^2}{(b + \cos t)^2} dt\right]$$

$$= (\sin A) \left[\int_o^{2\pi} \frac{(\sin t)^2}{b + \cos t} dt + b \frac{d}{db} \int_o^{2\pi} \frac{(\sin t)^2}{b + \cos t} dt\right]$$

$$= (\sin A) \left[2\pi(b - \sqrt{b^2 - 1}) + 2\pi b \left(1 - \frac{b}{\sqrt{b^2 - 1}}\right)\right]$$

Converting I_1, I_2 back to functionsof a gives:

$$h_1 = \frac{1}{\sqrt{a^2 + 1}} - 1 \qquad h_1 = -.293 \quad (a = 1)$$

$$\ell_1 = 0 \qquad \ell_1 = 0 \quad (a = 1)$$

$$m_1 = \frac{a^2 + 2}{a\sqrt{a^2 + 1}} - \frac{2}{a} \qquad m_1 = .121 \quad (a = 1) .$$

In selecting one of the systems (4.1a), that is, fixing a value of the parameter a, it should be noted that the (kidney-shaped) limit cycles show greater and greater fluctuations in velocity as a increases. Figure 6 shows the limit cycles for a = 1 and a = 5 with points marked at .1T intervals to give some indication of velocity. Experience with the (analytic) expansion for solutions of the kinetic system near the limit cycle suggests that irregular behavior, such as large fluctuations in velocity, decreases the range of validity of ϵ. Consequently, we fix a = 1 in the following numerical work. (Even in this case, values of on the order of .001 appear necessary to make $\phi_o(+\infty)$ a good approximation to the asymptotic phase $\hat{\phi}$.)

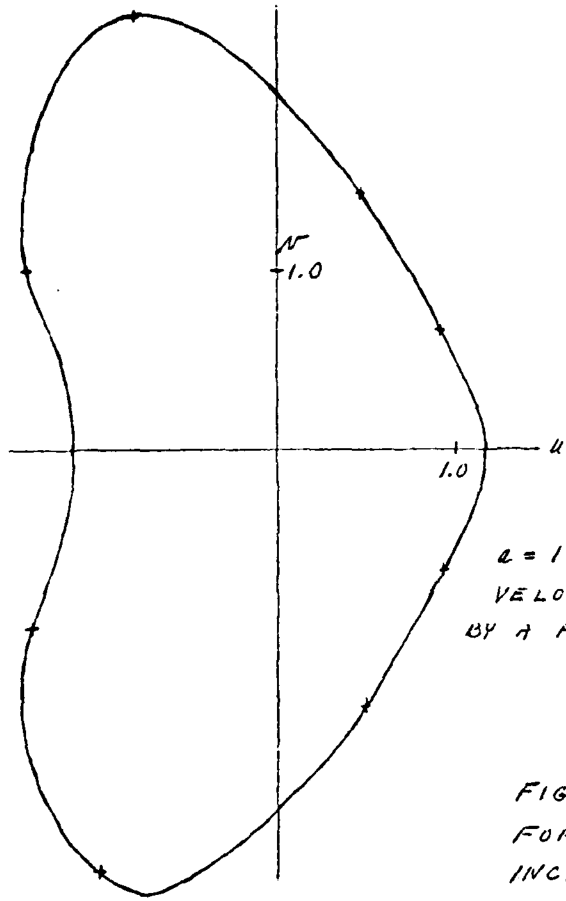
<u>Check I</u>. The period in ξ is taken to be P = 1. Initial data are

$$\begin{bmatrix} u(0,\xi) \\ v(0,\xi) \end{bmatrix} = \begin{bmatrix} R_o\ (\sin 2\pi\xi)\cos(\sin 2\pi\xi) \\ R_o\ (\sin 2\pi\xi)\sin(\sin 2\pi\xi) \end{bmatrix}$$

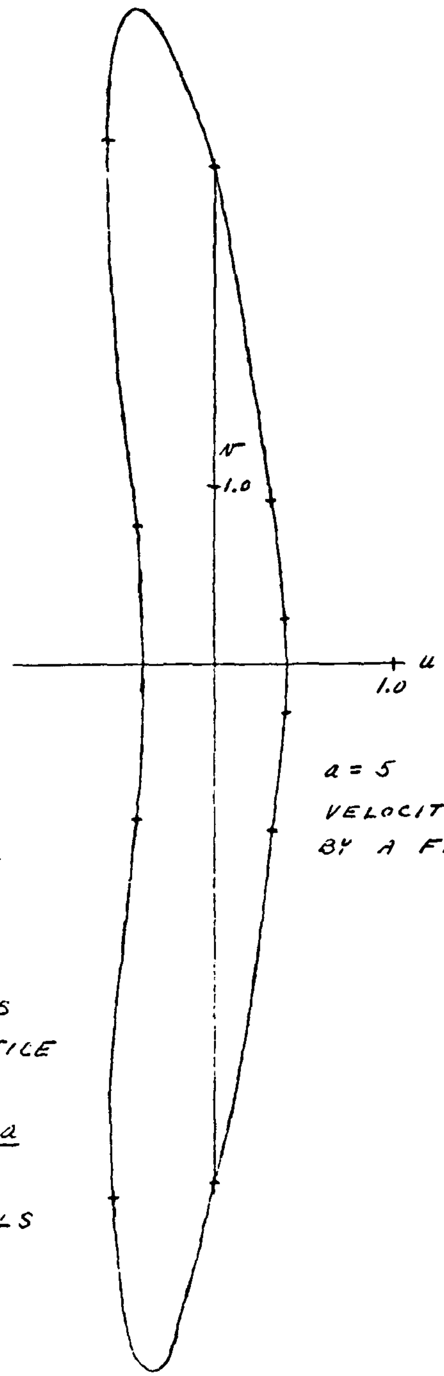
$$+\,\epsilon\tilde{B}(0,\xi)\begin{bmatrix} R_o^3\ (\sin 2\pi\xi)\cos(\sin 2\pi\xi) \\ R_o^3\ (\sin 2\pi\xi)\sin(\sin 2\pi\xi) \end{bmatrix},$$

that is, $\phi_o(0,\xi) = \sin(2\pi\xi)$, $B_1(0,\xi) = -\exp(+2a\sin(2\pi\xi))\,\tilde{B}(0,\xi)$.

Prediction I says the solution should evolve to a spatially homogeneous solution $(U(t+\hat{\phi}), V(t+\hat{\phi}))$ and that $\hat{\phi}$ is independent of $B_1(0,\xi)$. The solutions do in fact converge to a spatially homogeneous solution.



a = 1
VELOCITY VARIES
BY A FACTOR ~ 2.



a = 5
VELOCITY VARIES
BY A FACTOR ~ 7.

FIGURE 6. LIMIT CYCLES FOR EQUATION (4.1). NOTICE INCREASED VARIATION IN VELOCITY AS PARAMETER a INCREASES.
(MARKS AT TIME INTERVALS $\Delta t = T/10$.)

Comparison of $\hat{\phi}$ for initial conditions $\tilde{B}(0,\xi) \equiv 0$, .1 are given in Table 8A using $\Delta t = 2\pi/100$. The values are nearly the same in the two cases, as predicted. Table 8B shows the results when $\Delta t = 2\pi/600$. Notice that these uncorrected results for ϕ_{obs} are practically the same as ϕ_{num} with $\Delta t = 2\pi/100$. As in Section 3, the correction formula $\phi_{num} = \phi_{obs} -$ KPE (2.3) checks out.

Check II. Prediction II gives the approximate decay rate of the perturbation as $\exp(-(1+\alpha h_1)(\frac{2\pi}{P})^2 \epsilon\, t)$, so over each 2π-interval in t, the amplitude of the perturbation should be cut by approximately

$$\exp(-(1 - .293\alpha)\ 8\pi^3 \epsilon\ ).$$

The same initial data is used as in Check I. Defining the perturbation amplitude $A(t)$ as in (3.4), Table 9 sums up the observed amplitudes. The agreement with the predicted decay rate is excellent.

Check III. Now for Prediction III. The initial data are the same as in Check I, so the expected first-order approximation to $\hat{\phi}$ is

$$\phi_o(+\infty) = \frac{1 - .293\alpha}{.121\alpha}\ \ell n \left(I_o \left(\frac{.121\alpha}{1 - .293\alpha} \right) \right) .$$

The values of $\phi_o(+\infty)$ and ϕ_{num} are given in Table 10A. Unfortunately, the discrepancies are rather large (although still comparable to ϵ).

TABLE 8A

Check of Prediction I for (4.1)
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, $\phi_{num} = \phi_{obs} + .008$, carried to $t = 8\pi$

		$\epsilon\tilde{B}(0,\xi) \equiv 0$		$\epsilon\tilde{B}(0,\xi) \equiv .1$	
ϵ	α	ϕ_{obs}	ϕ_{num}	ϕ_{obs}	ϕ_{num}
.01	.9	.084	.092	.092	.100
.01	.0	.058	.064	.064	- .072
.01	- .9	- .011	- .003	- .005	+ .003

TABLE 8B

Check of Prediction I for (4.1) with smaller time steps
$\Delta\xi = .02$, $\Delta t = 2\pi/600$, carried to $t = 8\pi$

		$\epsilon\tilde{B}(0,\xi) \equiv 0$	$\epsilon\tilde{B}(0,\xi) \equiv .1$
ϵ	α	ϕ_{obs}	ϕ_{obs}
.01	.9	.090	.098
.01	.0	.064	.070
.01	- .9	- .005	.000

TABLE 9

Check of Prediction II for (4.1)

(predicted ratio = $\exp(-(1 - .293\alpha)8\pi^3\epsilon)$)

$\Delta\xi = .02$, $\Delta t = 2\pi/100$

	$\epsilon = .01$, $\alpha = .9$		$\epsilon = .01$, $\alpha = .5$		$\epsilon = .01$, $\alpha = .0$		$\epsilon = .01$, $\alpha = -.5$		$\epsilon = .01$ $\alpha = -.9$	
	predicted ratio = .161		predicted ratio = .120		predicted ratio = .084		predicted ratio = .058		predicted ratio = .044	
t	A(t)	ratio	A(t)	ratio	A(t)	ratio	A(t)	ratio	A(t)	ratio
0	2.000	---	2.000	---	2.000	---	2.000	---	2.000	---
2π	.286	.14	.241	.12	.184	.09	.134	.07	.101	.05
4π	.041	.14	.029	.12	.015	.08	.008	.06	.005	.05
6π	.006	.14	.003	.10	.001	.07	.000	---	.000	---
8π	.000	---	.000	---	.000	---	.000	---	.000	---

TABLE 10A

Check of Prediction III for (4.1)
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, carried to $t = 8\pi$

ϵ	α	ϕ_{num}	$\phi_o(+\infty)$	discrepancy
.01	.9	.093	.037	.056
.01	.5	.085	.018	.067
.01	.0	.066	.000	.066
.01	-.5	.034	-.013	.047
.01	-.9	-.003	-.023	.020

TABLE 10B

Check of Prediction III for (4.1)
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, carried to $t = 16\pi$

ϵ	α	ϕ_{num}	$\phi_o(+\infty)$	discrepancy
.005	.9	.073	.037	.036
.005	.5	.064	.018	.046
.005	.0	.045	.000	.045
.005	-.5	.019	-.013	.032
.005	-.9	-.007	-.023	.016

TABLE 10C

Check of Prediction III for (4.1)
$\Delta\xi = .02$, $\Delta t = 2\pi/100$, carried to $t = 32\pi$.

ϵ	α	ϕ_{num}	$\phi_o(+\infty)$	discrepancy
.0025	.9	.061	.037	.024
.0025	.5	.047	.018	.029
.0025	.0	.028	.000	.028
.0025	-.5	.007	-.013	.020
.0025	-.9	-.010	-.023	.013

The experience with discrepancies in the λ-ω system case suggests that this system may have a relatively large $O(\epsilon)$-term, which is the source of the discrepancies. To test this hypothesis, runs with smaller values of ϵ (from $\epsilon = .01$ to .005 to .0025) are given in Tables 10B, C. Notice that cutting ϵ in half forces carrying the solution twice as far in t, because it evolves to a spatially homogeneous solution only half as fast. Each time ϵ is reduced by half, the discrepancy is reduced to roughly 2/3 its previous value. The reason the discrepancy is not cut to 1/2 its previous value is most likely numerical error accumulating over the longer and longer integration times required.

The numerical results clearly show $|\phi_{num} - \phi_o(+\infty)| = O(\epsilon)$, which agrees with Prediction III. The trends in Tables 10A-C indicate that $\phi_o(+\infty)$ will be a good approximation to $\hat{\phi}$ for $\epsilon < .001$. No attempt was made to investigate ϕ_{num} for such small values of ϵ: for $\epsilon = .0025$, integration to $t = 32\pi$ was necessary for a spatially homogeneous solution and at least 80π would be necessary for $\epsilon = .001$).

The numerical results in this case have directly confirmed Predictions I and II and indirectly confirmed Prediction III.

Numerical Methods for Reaction-Diffusion Equations

This section discusses numerical methods of solving the (vector) reaction-diffusion equations

$$\underset{\sim}{u}_t = F(\underset{\sim}{u}) + K\underset{\sim}{u}_{xx}, \quad K \text{ positive-definite matrix.} \tag{5.1}$$

For simplicity, only one space variable is considered. Periodic boundary conditions (on $0 \leq x \leq 1$) will be used when boundary conditions are relevant. The three methods to be considered are

$(u_n^m = \underset{\sim}{u}(m\Delta x,\ n\Delta t))$

<u>Explicit</u> $$\frac{1}{\Delta t}(u_{n+1}^m - u_n^m) = \frac{1}{\Delta x^2} K (u_n^{m+1} - 2\, u_n^m + u_n^{m-1}) + F(u_n^m); \qquad (5.2a)$$

<u>Crank-Nicholson</u> $$\frac{1}{\Delta t}(u_{n+1}^m - u_n^m) = \frac{1}{2\Delta x^2} K \, [(u_{n+1}^{m+1} - 2u_{n+1}^m + u_{n+1}^{m-1}) \qquad (5.2b)$$

$$+ (u_n^{m+1} - 2u_n^m + u_n^{m-1})] + F(\tfrac{1}{2}(u_{n+1}^m + u_n^m));$$

<u>Lees'</u> $$\frac{1}{\Delta t}(u_{n+1}^m - u_n^m) = \frac{1}{2\Delta x^2} K \, [(u_{n+1}^{m+1} - 2\, u_{n+1}^m + u_{n+1}^{m-1}) \qquad (5.2c)$$

$$+ (u_n^{m+1} - 2u_n^m + u_n^{m-1})] + F(\tfrac{3}{2}\, u_n^m - \tfrac{1}{2}\, u_{n-1}^m);$$

<u>Modified Lees'</u> $$\frac{1}{\Delta t}(u_{n+1}^m - u_n^m) = \frac{1}{2\Delta x^2} K \, [(u_{n+1}^{m+1} - 2u_{n+1}^m + u_{n+1}^{m-1}) \qquad (5.2d)$$

$$+ (u_n^{m+1} - 2u_n^m + u_n^{m-1})]$$

$$+ \tfrac{3}{2} F(u_n^m) - \tfrac{1}{2} F(u_n^m) \; .$$

The standard results on accuracy and numerical stability for these methods and some comments on their programming will be given in this section. The next section discusses results obtained on the nonlinear stability of these finite difference methods.

First, consider accuracy. For the explicit method, expanding the difference equation around $(x,t) = (m\Delta x, n\Delta t)$ gives $(u = u_n^m)$

$$u_t = K\,u_{xx} + F(u) + [-\frac{1}{2}u_{tt}\,\Delta t + \frac{1}{12}K\,u_{xxxx}\,\Delta x^2 + O(\Delta t^2, \Delta x^4)]. \tag{5.3a}$$

Roughly speaking, solutions of the finite difference equations solve this nonhomogeneous form of (5.1). On a fixed, bounded (x,t)-domain, we expect the solution of the finite difference equations to differ from the actual solution (5.1) by an amount proportional to the nonhomogeneous terms, so the accuracy of the explicit method is $O(\Delta t, \Delta x^2)$.

For the Crank-Nicolson, Lees', and modified Lees' methods, expansions of (5.2b,c,d) around $x,t = m\Delta x, (n + \frac{1}{2})\Delta t$ give

$$u_t = Ku_{xx} + F(u) + O(\Delta t^2, \Delta x^2) \tag{5.3b}$$

and these three methods have accuracy $O(\Delta t^2, \Delta x^2)$.

A very curious phenomenon occurs in the application of finite difference schemes to real problems. A finite difference equation in

Δx, Δt is consistent with a PDE if the difference formula converges to the PDE as $\Delta x, \Delta t \to 0$ (for instance, the equations (5.2a-d) are all consistent with (5.1)). One would expect that if (1) a given finite difference equation is consistent with a PDE and (2) solutions (for fixed initial data) of the difference equation are generated as $\Delta x, \Delta t \to 0$, then those solutions would approach a solution of the PDE. But this is not necessarily true: the finite difference solutions may not even remain bounded, let alone converge to the continuous solutions!

If the solutions of a finite difference equation remain bounded as $\Delta x, \Delta t \to 0$, then the scheme is said to be (numerically) stable. The importance of this property is shown by a theorem of Lax: for a PDE and a consistent finite difference equation (and certain conditions), solutions of the finite difference equation converge to solutions of the PDE if and only if the difference scheme is stable (see Richtmeyer and Morton, 1967).

Generally, a finite difference scheme is said to be stable if it is stable when applied to a linear PDE with constant coefficients. The finite difference solutions can be found exactly in such cases by the finite analogue of Fourier analysis, and boundedness determined directly. Some results are known for linear systems with variable coefficients, but very little is known about numerical stability of finite difference schemes applied to nonlinear equations.

The idea of numerical stability for the linear case will be illustrated here for scalar u. Some of this material will be used in deriving the nonlinear stability results of the next two sections.

In the following, (5.1) is taken as a scalar equation for simplicity and $F(u) = -gu$, g constant. Integration is over a finite x,t-domain $0 \leq x \leq 1$, $0 \leq t \leq T$; the finite difference steps are $\Delta x = 1/M$, $\Delta t = T/N$; u_n^m corresponds to $u(m\Delta x, n\Delta t)$, $0 \leq m \leq M$, $0 \leq n \leq N$. Periodic boundary conditions mean $u_n^0 = u_n^M$, all n. Variables u_k refer to the whole vector $(u_k^0, u_k^1, \ldots)$; sometimes u will be used to refer to refer to the vector $(u^0, u^1, \ldots)$. Setting $\lambda = K\Delta t/\Delta x^2$, the four methods in (5.2) reduce to:

<u>Explicit</u> $\quad u_{n+1}^m = u_n^m + \lambda(u_n^{m+1} - 2u_n^m + u_n^{m-1}) - g\Delta t \;\; u_n^m$, u_o given. $\quad$ (5.4a)

<u>Crank-Nicolson</u> $\quad$ (5.4b)

$$u_{n+1}^m = u_n^m + \frac{\lambda}{2}\,[(u_{n+1}^{m+1} - 2u_{n+1}^m + u_{n+1}^{m-1})$$

$$+ (u_n^{m+1} - 2u_n^m + u_n^{m-1})]$$

$$- \frac{1}{2}\, g\Delta t\; (u_{n+1}^m + u_n^m),\quad u_o \text{ given.}$$

<u>Lees' and Modified Lees'</u> $\quad$ (5.4c)

$$u_{n+1}^m = u_n^m + \frac{1}{2}\lambda\,[(u_{n+1}^{m+1} - 2u_{n+1}^m + u_{n+1}^{m-1}) + (u_n^{m+1} - 2u_n^m + u_n^{m-1})]$$

$$- \frac{g}{2}\,\Delta t\; (3\,u_n^m - u_{n-1}^m),\quad u_o,\ u_1 \text{ given.}$$

Notice that Lees' and the modified Lees' methods reduce to the same scheme for linear F(u).

These equations can be solved by a discrete analog of Fourier series. A vector u, considered as a function of m = 0, 1, ..., M-1, is expanded in terms of the functions

$$\frac{1}{\sqrt{M}}\exp\left(+2\pi i\ \frac{pm}{M}\right),\ p = 0, 1, 2, \ldots, M-1, \tag{5.5a}$$

and these are orthogonal in the sense that

$$\sum_{m=0}^{M-1} \frac{1}{M}\ \exp\left(+2\pi i\ \frac{pm}{M}\right) \exp\left(-2\pi i\ \frac{qm}{M}\right) = \begin{cases} 1 \text{ if } p = q \\ 0 \text{ if } p \neq q,\ 0 \leq p,\ q \leq M-1. \end{cases} \tag{5.5b}$$

The expansion has the form

$$u^m = \sum_{p=0}^{M-1} \alpha^p \frac{1}{\sqrt{M}}\ \exp\left(+2\pi i\ \frac{pm}{N}\right) \tag{5.5c}$$

$$\text{where } \alpha^p = \sum_{m=0}^{M-1} u^m \frac{1}{\sqrt{M}} \exp\left(-2\pi i\ \frac{pm}{M}\right).$$

It is interesting to obtain these results from another point of view. Notice the operator $u^m - \frac{\mu}{2}(u^{m+1} - 2u^m + u^{m-1}) \equiv (I - \frac{\mu}{2}(E - 2I + E^{-1}))\,u$ occurs in both equations of (5.4) (E is the shift operator, $Eu^{M-1} = u^0$ by periodicity). This operator corresponds to a symmetric (almost tridiagonal) matrix. The eigenvectors v_p are

$$v_p^m = \frac{1}{\sqrt{M}} \exp\left(+ 2\pi i \frac{pm}{M}\right), \quad p = 0, 1, \ldots, M-1, \tag{5.6a}$$

$$\left(I - \frac{\mu}{2}(E - 2I + E^{-1})\right)v_p = \left[1 + 2\mu\left(\sin\left(\frac{p\pi}{M}\right)\right)^2\right]v_p. \tag{5.6b}$$

It follows immediately from matrix theory for symmetric matrices that the eigenvectors are orthogonal with respect to the inner product and corresponding norm:

$$(u,v) = \sum_{m=0}^{M-1} u^m \; \overline{v^m}, \tag{5.7}$$

$$||u||_2 = \left(\sum_{m=0}^{M-1} |u^m|^2\right)^{1/2}.$$

The orthogonality of the eigenvectors is then (5.5b).

Direct solutions of (5.4) can be obtained by the finite difference form of separation of variables. Set

$$u_n^m = \sum_{p=0}^{M-1} \alpha_n^p \, v_p^m \tag{5.8a}$$

and substitute into (5.4a) to obtain a recursion formula for the Fourier coefficients

$$\alpha_{n+1}^p = \left[1 - 4\lambda\left(\sin\frac{p\pi}{M}\right)^2 - g\Delta t\right]\alpha_n^p. \tag{5.8b}$$

Substitution into (5.4b,c) gives recursion formulas for the Fourier coefficients

$$\alpha_{n+1}^{p} = \frac{1 - 2\lambda(\sin\frac{p\pi}{M})^2 - \frac{1}{2}g\,\Delta t}{1 + 2\lambda(\sin\frac{p\pi}{M})^2 + \frac{1}{2}g\,\Delta t}\,\alpha_n^p, \tag{5.8c}$$

$$\alpha_{n+1}^{p} = \frac{1 - 2\lambda(\sin\frac{p\pi}{M})^2 - \frac{3}{2}g\,\Delta t}{1 + 2\lambda(\sin\frac{p\pi}{M})^2}\,\alpha_n^p$$

$$+ \frac{\frac{1}{2}g\,\Delta t}{1 + 2\lambda(\sin\frac{p\pi}{M})^2}\,\alpha_{n-1}^p. \tag{5.8d}$$

In (5.8b), notice that if the coefficient of α_n^p has magnitude greater than 1 (which can happen if $|\,1 - 4\lambda - g\Delta t\,| \geq 1 + \epsilon,\ \epsilon > 0$), then the α_n^p will blow up as $\Delta t \rightarrow 0$ because the final coefficient is

$$\alpha_N^p = (1 - 4\lambda(\sin\frac{p\pi}{M})^2 - g\,\frac{T}{N})^N\,\alpha_0^p \quad \text{and} \quad N \rightarrow +\infty\,.$$

The $g\,\Delta t$ term may introduce some mild growth over $0 \leq t \leq T$, but does not lead to unboundedness if $|(1 - 4\lambda)| > 1$. The result is the <u>conditional stability restriction for the explicit method</u>

$$|1 - 4\lambda| \leq 1 \quad \text{or} \quad \frac{K\,\Delta t}{\Delta x^2} \leq \frac{1}{2}\,. \tag{5.9}$$

In (5.8c), the coefficient of α_n^p is always smaller than 1 in magnitude as long as the relatively minor condition $1 \pm g\,\Delta t > 0$ holds, so the Crank-Nicolson method is said to be unconditionally stable.

In (5.8d), notice the recursion formula for $g = 0$ becomes

$$\alpha_{n+1}^p = \frac{1 - 2\lambda(\sin \frac{p\pi}{M})^2}{1 + 2\lambda(\sin \frac{p\pi}{M})^2}\ \alpha_n^p \tag{5.10}$$

and the coefficient of α_n^p always has magnitude ≤ 1 (since $|(1 - 2\lambda x)/(1 + 2\lambda x)| \leq 1$ for $0 \leq x < \infty$), so solutions in this case never blow up. For $g \neq 0$, this growth factor is only perturbed by $g\Delta t$, which may add some exponential growth in t but does not lead to unbounded solutions as $N \to \infty$. Consequently, the Lees' and modified Lees' methods are unconditionally stable.

It should be pointed out that for linear equations stability seems to be related only to the wave length of the Fourier components--amplitude is unimportant. In the nonlinear case amplitude and wavelength both are involved in stability. Some basis for this can be seen in the gu-term in (5.4) by the above analysis; the stability results assume $g\Delta t$ is small. For the nonlinear case g will be a function of u, and for a fixed small Δt, $g(u)\Delta t$ may be small (with stability expected) for small amplitude u, and $g(u)\Delta t$ may become large (with instability expected) for large amplitude u ($\Delta t, \Delta x$ held fixed). Such an example will be given in the next section.

The basic numerical problem of the first half of this chapter was the solution of

$$u_t = F(u,v) + \epsilon_1 u_{xx}$$

$$v_t = G(u,v) + \epsilon_2 v_{xx} \tag{5.11}$$

with periodic boundary conditions on $0 \leq x \leq 1$, and F, G nonlinear. The explicit method is undesirable because the stability restriction (5.9) forces Δt to be extremely small. (The method is usable, however; Fitzhugh used it to compute traveling wave solutions of the Fitzhugh-Nagumo equations, a reaction-diffusion system arising in modeling the nerve impulse (Rinzel, 1977).) The Crank-Nicolson method requires the solution of a nonlinear system of equations because of the $F(\frac{1}{2}(u^m_{n+1} + u^m_n))$ term. Lees' and the modified Lees' methods are equivalent in accuracy and stability; Lees' method was used in the calculations of the first half of this chapter.

In using Lees' method expressions for $F(u,v)$, $G(u,v)$, $u(x,0)$, $v(x,0)$ were needed as well as specifications of ϵ_1, ϵ_2, Δt, Δx. The usual values taken were $\Delta x = .02$ (sometimes .01), $\Delta t = 2\pi/100$ or $2\pi/600$, and ϵ_1, ϵ_2 in the range .0025-.0100. The usual run had 400-800 time steps, although some runs went to 4800 time steps. Trial runs comparing numerical and exact solutions (specifically, λ-ω traveling waves) were compatible with the theoretical error $O(\Delta x^2, \Delta t^2)$. No signs of numerical instability ever occurred. When the runs concerned spatial perturbations of the limit cycle, the major part of the error occurred as a phase shift--the procedure for eliminating a considerable portion of this error by applying the finite difference method to the kinetic equations alone has been discussed in detail in Section 2 (which made possible the rather large time steps $\Delta t = 2\pi/100$).

Since Lees' and the modified Lees' methods are implicit it is necessary to solve an MxM linear system at each time step. For periodic boundary conditions, the coefficient matrix has the form

$$\begin{bmatrix} 1+c_i & -\frac{1}{2}c_i & 0 & 0 & \cdots & 0 & -\frac{1}{2}c_i \\ -\frac{1}{2}c_i & 1+c_i & -\frac{1}{2}c_i & 0 & & 0 & 0 \\ 0 & -\frac{1}{2}c_i & 1+c_i & & & & \\ 0 & 0 & & & & & \\ & \cdots & & & & \cdots & \\ 0 & 0 & & & & 1+c_i & -\frac{1}{2}c_i \\ -\frac{1}{2}c_i & 0 & 0 & \cdots & & -\frac{1}{2}c_i & 1+c_i \end{bmatrix}, \quad c_i = \frac{\epsilon_i \, \Delta t}{\Delta x^2} \; . \tag{5.12}$$

This matrix has the same form as the operator considered in (5.6) ($\mu = c_i$) and its eigenvalues are between 1 and $1 + 2c_i$. It can be solved by Gaussian elimination almost as efficiently as a tridiagonal system; the idea is to take advantage of sparseness of the matrix and use only the 3 main diagonals, the last row, and the last column.* For some reason this inversion routine (in double precision) for the 50x50 system gives exponential underflow errors for ϵ_i above .01. No investigation of this was carried out since multiple checks showed no programming error and only small ϵ_i-values were of interest.

Runs of the same initial data for Lees' and the modified Lees' methods agreed to 3 significant digits, in accord with the error.

Nonlinear Numerical Stability: Geometric Approach

In this section we adapt the geometric proofs of boundedness for solutions of reaction-diffusion equations (Chueh, Conley, and Smoller (1977), discussed in Chapter I) to the finite difference schemes (5.2). For simplicity only the scalar case is considered, but some comments on systems will be made at the end of the section. The basic assumption is

$$\text{there exist } A_1, A_2, A_1 < A_2, \text{ such that } F(A_1) > 0 \text{ and } F(A_2) < 0. \qquad (6.1)$$

This assumption makes the interval $A_1 \leq u \leq A_2$ a <u>positively-invariant region</u> for the equation (5.1), that is, if F(u) has this property, then the results of Chueh, Conley, and Smoller (1977) show that $A_1 \leq u(x,0) \leq A_2$ initially implies $A_1 \leq u(x,t) \leq A_2$ for all $t \geq 0$ (or as long as the solution remains smooth).

*Although the eigenvectors and hence an explicit inverse can be calculated from (5.6), I think elimination is quicker because the inverse is a full matrix.

This section shows that if initial data u_0 (or u_0, u_1) for the finite difference methods (5.2) start in the region $[A_1, A_2]$ and that $\Delta t = O(\Delta x^2)$ and (6.1) holds, then the finite difference solution stays in the region $[A_1, A_2]$ for all n. (The $\Delta t = O(\Delta x^2)$ condition is the best that can be expected for the explicit method, but one hopes for something better for the other three implicit methods. Stronger results can, in fact, be derived by direct estimates given in the next section, but considerably more work is required.)

The geometric approach is nicely illustrated in the following theorem on stability of the explicit method.

Theorem 1. Assume (a) F(u) in the explicit method (5.2a) satisfies (6.1),

(b) the periodic initial data u_0 satisfy

$$A_1 \le u_o^m \le A_2,$$

(c) $\Delta t \le \dfrac{\Delta x^2}{2K + B\,\Delta x^2}$, where

$$B \ge \sup_{A_1 \le u \le A_2} \frac{F(u)}{A_1 - u}, \ \sup_{A_1 \le u \le A_2} \frac{F(u)}{A_2 - u} .$$

Then $A_1 \le u_n^m \le A_2$ for all n.

Proof: First notice that a finite B exists because $F(u)/A_1-u) \to -\infty$ as $u \to A_1^+$ by (6.1); similarly for $F(u)/(A_2-u)$.

Let $\hat{n}$ be that value of n such that $A_1 \leq u_{\hat{n}}^{m} \leq A_2$ for all m, but there exists $\hat{m}$ such that $A_2 < u_{\hat{n}+1}^{\hat{m}}$; without loss of generality $A_{\hat{n}+1}^{\hat{m}}$ is a maximum over $A_{\hat{n}+1}^{m}$. From (5.2),

$$u_{\hat{n}+1}^{\hat{m}} - u_{\hat{n}}^{\hat{m}} = \frac{K\Delta t}{\Delta x^2} \left(u_{\hat{n}}^{\hat{m}+1} - 2\, u_{\hat{n}}^{\hat{m}} + u_{\hat{n}}^{\hat{m}-1}\right) + F(u_{\hat{n}}^{\hat{m}})\Delta t.$$

Replacing $u_{\hat{n}}^{\hat{m}}$ by u, notice that

$$u_{\hat{n}+1}^{\hat{m}} - u_{\hat{n}}^{\hat{m}} > A_2 - u,$$

$$u_{\hat{n}}^{\hat{m}+1} - 2\, u_{\hat{n}}^{\hat{m}} + u_{\hat{n}}^{\hat{m}-1} \leq A_2 - 2u + A_2,$$

consequently,

$$A_2 - u < 2\, \frac{K\Delta t}{\Delta x^2} (A_2 - u) + F(u)\Delta t,$$

$$\text{or} \quad 1 < \Delta t \left(\frac{2K}{\Delta x^2} + \frac{F(u)}{A_2 - u} \right) .$$

But this inequality contradicts hypothesis (c) on Δt, by the definition of B.

If $u_{\hat{n}+1}^{\hat{m}} < A_1$, a similar argument applies. QED.

To attempt a similar result for the Crank-Nicolson, Lees', and modified Lees' methods, notice all three can be written in the form

$$u_{n+1}^{m} - u_{n}^{m} = \frac{K\Delta t}{2\Delta x^2}\left[(u_{n+1}^{m+1} - 2\,u_{n+1}^{m} + u_{n+1}^{m-1}) + (u_{n}^{m+1} - 2\,u_{n}^{m} + u_{n}^{m-1})\right]$$

$$+ G\,(u_{n+1}^{m},\ u_{n}^{m},\ u_{n-1}^{m})\Delta t. \tag{6.2}$$

Again take $\hat{n}$ such that $u_{\hat{n}+1}^{\hat{m}}$ is a maximum over $u_{\hat{n}+1}^{m}$, that $u_{\hat{n}+1}^{\hat{m}} > A_2$, and that $A_1 \le u_{\hat{n}}^{m},\ u_{\hat{n}-1}^{m}, \le A_2$ for all m. Writing u,v for $u_{\hat{n}}^{\hat{m}},\ u_{\hat{n}-1}^{\hat{m}}$ and using

$$u_{\hat{n}+1}^{\hat{m}} - u_{\hat{n}}^{\hat{m}} > A_2 - u,$$

$$u_{\hat{n}}^{\hat{m}-1} - 2\,u_{\hat{n}}^{\hat{m}} + u_{\hat{n}}^{\hat{m}-1} \le A_2 - 2u + A_2, \tag{6.3}$$

$$u_{\hat{n}+1}^{\hat{m}+1} - 2\,u_{\hat{n}+1}^{\hat{m}} + u_{\hat{n}+1}^{\hat{m}-1} \le 0 \text{ (since } u_{\hat{n}+1}^{\hat{m}} \text{ is a maximum)},$$

we conclude from (6.2) that

$$1 < \Delta t\left(\frac{K}{\Delta x^2} + \frac{G(A_2,\ u,\ v)}{A_2 - u}\right). \tag{6.4a}$$

Similarly, if $u_{\hat{n}+1}^{\hat{m}} < A_1$ and $u_{\hat{n}+1}^{\hat{m}}$ is a minimum, then

$$1 < \Delta t\left(\frac{K}{\Delta x^2} + \frac{G(A_1,\ u,\ v)}{A_1 - u}\right). \tag{6.4b}$$

For Crank-Nicolson, notice that $G = F(\frac{1}{2}(A_2 + u))$ or $F(\frac{1}{2}(A_1 + u))$, $A_1 \leq u \leq A_2$; for Lees', $G = F(\frac{3}{2} u - \frac{1}{2} v)$ with $A_1 \leq u, v \leq A_2$; for modified Lees', $G = \frac{3}{2} F(u) - \frac{1}{2} F(v)$ with $A_1 \leq u, v \leq A_2$. Both (6.4a) and (6.4b) would be impossible if there existed a finite B such that

$$B \geq \sup_{A_1 \leq u, v \leq A_2} \frac{G(A_2,u,v)}{A_2-u}, \quad \sup_{A_1 \leq u, v \leq A_2} \frac{G(A_1,u,v)}{A_1-u}. \tag{6.5}$$

and Δt, Δx satisfied

$$1 \geq \Delta t \left(\frac{K}{\Delta x^2} + B\right). \tag{6.6}$$

The basic problem is whether a finite B satisfying (6.5) exists, and we consider conditions under which it would exist for the different definitions of G in the 3 methods.

In the Crank-Nicolson case, (6.1) alone is sufficient to insure the existence of an upper bound B(as $u \to A_2^-$, $F(\frac{1}{2}(A_2+u))/(A_2-u) \to -\infty$ and as $u \to A_1^+$, $F(\frac{1}{2}(A_1+u))/(A_1-u) \to -\infty$ also).

The case for Lees' method is a little more complicated. Obviously assumptions must be put on F(w) for w outside the invariant region $A_1 \leq w \leq A_2$, for instance,

$$F(w) < 0 \quad \text{for} \quad A_2 \leq w \leq A_2 + \frac{1}{2}(A_2 - A_1) \tag{6.7}$$

$$F(w) > 0 \quad \text{for} \quad A_1 - \frac{1}{2}(A_2 - A_1) \leq w \leq A_1.$$

Consequently, for each v with $A_1 \leq v \leq A_2$, $F(\frac{3}{2}u - \frac{1}{2}v)/(A_2 - u) \to -\infty$ as $u \to A_2^-$ in (6.5) and a finite upper bound exists; similarly for $u \to A_1^+$.

For the modified Lees' method no condition outside the region is necessary. Instead a "flatness" condition on F(w) for w in $[A_1, A_2]$ is sufficient (together with (6.1)):

$$3F(A_1) > F(w) > 3F(A_2) \text{ for } A_1 \leq w \leq A_2. \tag{6.8}$$

Then for each v, $A_1 \leq v \leq A_2$, $(\frac{3}{2}F(u) - \frac{1}{2}F(v))/(A_2 - u) \to -\infty$ as $u \to A_2^-$ and a finite upper bound exists; similarly for the other case with $u \to A_1^+$.

Summarizing the results for these three cases gives:

Theorem 2. Let $F(u)$ satisfy (6.1) and initial data u_0 (and u_1 for Lees', modified Lees' methods) satisfy $A_1 \leq u_0^m, u_1^m, \leq A_2$. Then:

(a) there exists a finite constant B such that when Δx, Δt satisfy (6.6), then Crank-Nicolson solutions satisfy $A_1 \leq u_n^m \leq A_2$ for all n;

(b) if $F(u)$ satisfies (6.7), there exists a finite constant B such that when Δx, Δt satisfy (6.6), then Lees' method solutions satisfy $A_1 \leq u_n^m \leq A_2$ for all n;

(c) if $F(u)$ satisfies (6.8), there exists a finite constant B such that when Δx, Δt satisfy (6.6), then modified Lees' method solutions satisfy $A_1 \leq u_n^m \leq A_2$ for all n.

The restriction $\Delta t = O(\Delta x^2)$ here is rather restrictive in comparison with the unconditional stability of these methods for the linear case; on the other hand, a stronger result (that the solutions are actually bounded by a constant) is obtained. Something better than $\Delta t = O(\Delta x^2)$ should be obtainable if one goes to direct estimates, and this approach is used in the next section.

Generalization of these arguments to systems should be relatively straightforward. For K positive-definite, Chueh, Conley, and Smoller (1977) show the positively-invariant region to be a "box" with sides which are hyperplanes orthogonal to the eigenvectors of K. The condition on the (vector) function F(u) is that the direction field for F point strictly inwards on the surface of the box--the direct generalization of (6.1). See Chapter I for a more detailed discussion of their results.

The quantity B in Theorems 1 and 2 measures, roughly speaking, the strength of the nonlinearity--the larger B, the smaller Δt (or Δx) must be. We shall end this section with an example showing how the nonlinear term can act to make solutions obtained using Lees' method blow up.

Take the equation

$$u_t = K\, u_{xx} - u^3 \tag{6.9}$$

and notice that any solution should decay to 0 and that any interval $[A_1, A_2]$ with $A_1 < 0 < A_2$ is a positively-invariant region. Lees' method has the form ($\lambda = K\Delta t/2\Delta x^2$)

$$u^m_{n+1} - u^m_n = \lambda \left[(u^{m+1}_{n+1} - 2\, u^m_{n+1} + u^{m-1}_{n+1}) + (u^{m+1}_n - 2\, u^m_n + u^{m-1}_n)\right]$$

$$- \Delta t \left(\frac{3}{2}\, u^m_n - \frac{1}{2}\, u^m_{n-1}\right)^3 \tag{6.10}$$

This difference equation has a solution of the form

$$u^m_n = (-1)^{n+m}\, A_n, \tag{6.11a}$$

$$A_{n+1} = \frac{4\lambda - 1}{4\lambda + 1} A_n + \frac{\Delta t}{4\lambda + 1} \left(\frac{3}{2} A_n + \frac{1}{2} A_{n-1}\right)^3, \tag{6.11b}$$

with A_0, A_1 given.

Notice that if A_n, A_{n-1} are small, the nonlinear term is very small and solutions $A_n \to 0$ as $n \to +\infty$. But, if the initial amplitude is increased, the solution $A_n \to +\infty$ as $n \to +\infty$. Specifically, assume $0 \leq A_0 \leq A_1$ and that

$$\Delta t \; \frac{27}{8} A_1^2 > 2. \tag{6.12}$$

Then in the nonlinear term,

$$\Delta t \left(\frac{3}{2} A_1 + \frac{1}{2} A_o\right)^3 \geq \Delta t \left(\frac{3}{2} A_1\right)^3 > 2A_1,$$

so $$A_2 > \frac{4\lambda - 1}{4\lambda + 1} A_1 + \frac{2}{4\lambda + 1} A_1 = A_1.$$

Since $A_2 > A_1$, then A_2 also satisfies (6.12), so $A_3 > A_2$, etc. Obviously the process accelerates once started and A_n increases to $+\infty$ as $n \to +\infty$.

Here Δt, Δx are assumed fixed. The example shows that when amplitudes are small compared to Δt, solutions decay to 0 as n increases, but when amplitudes are large compared to Δt, solutions blow up as n increases. The comparison between the amplitude and Δt is given by (6.12).

Nonlinear Numerical Stability: Direct Estimates

This section considers the nonlinear stability of Lees' and the modified Lees' methods by obtaining explicit bounds on the solutions. For simplicity, only the scalar case--with periodic boundary conditions--of (5.1) is considered. That is, we are solving ($\lambda = \Delta t K/\Delta x^2$; $G(u,v) = F(\frac{3}{2}u - \frac{1}{2}v)$ or $\frac{3}{2}F(u) - \frac{1}{2}F(v)$):

$$u^m_{n+1} - \frac{\lambda}{2}(u^{m+1}_{n+1} - 2u^m_{n+1} + u^{m-1}_{n+1}) = u^m_n + \frac{\lambda}{2}(u^{m+1}_{n+1} - 2u^m_{n+1} + u^{m-1}_{n+1})$$

$$+ \Delta t\, G(u^m_n, u^m_{n-1}). \tag{7.1}$$

with u_0, u_1 given. The main result of this section is to give conditions on the initial data u_0, u_1 which insure that solutions of the difference scheme (7.1) remain bounded as $\Delta x, \Delta t \to 0$ (unconditionally) on the given domain.

First, pick some large $A > 0$ which will serve as the bound on our solutions (eventually). Given A, define B_1 and B_2 as follows:

$$|a|, |b| \leq A \text{ implies } |G(a,b)| \leq B_1, \tag{7.2}$$

$$|a_i|, |b_i| \leq A \text{ implies } |G(a_1,b_1) - G(a_2,b_2)|$$

$$\leq B_2 \left(|a_2-a_1|^2 + |b_2-b_1|^2\right)^{1/2}.$$

We estimate the "drift" of a solution by observing its mean. Given a vector u, define its mean value $\hat{u}$ by

$$\hat{u} = \frac{1}{M} \sum_{m=0}^{M-1} u^m. \tag{7.3}$$

By summing (7.1) over all m and using the periodicity condition $u^M = u^0$, we get an equation for the mean value:

$$\hat{u}_{n+1} = \hat{u}_n + \frac{1}{M} \sum_{m=0}^{M-1} G(u_n^m, u_{n-1}^m)\, \Delta t, \tag{7.4}$$

so $\quad |\hat{u}_{n+1}| \leq |\hat{u}_n| + B_1 \Delta t.$

We can now state the main result:

Theorem 3. Let the domain be $0 \leq x \leq 1$, $0 \leq t \leq T$ with $\Delta x = 1/M$ and $\Delta t = T/N$; let u_n be the solution of the finite difference scheme (7.1) on this domain. Let $A > 0$ be given and B_1, B_2 defined by A as in (7.2). Assume there exist A_0, $A_1 > 0$ be such that

$$A_0 + \frac{1}{2} \exp(\sqrt{2}\, B_2 T) A_1 + B_1 T \leq A. \tag{7.5}$$

If $\|u_0\|_\infty$, $\|u_1\|_\infty \leq A_0$ and $\|Du_0\|_2$, $\|Du_1\|_2 \leq A_1/\sqrt{M}$, then $\|u_n\|_\infty \leq A$ for all sufficiently large M, N.

NOTE: (1) The positive constants A_0, A_1 exist if and only if $B_1 T < A$.

(2) Du represents the difference vector with components $u^{m+1} - u^m$. The condition on $||Du_0||_2$, $||Du_1||_2$ may look restrictive at first glance, but notice

$$||Du||_2 = \left(\sum_{m=0}^{M-1} |u^{m+1} - u^m|^2 \right)^{1/2}$$

$$\sim \left(\sum_{m=0}^{M=1} (u_x(m\, x))^2\, x^2 \right)^{1/2} \quad \left(\int_0^1 u_x^2\, dx \right)^{1/2} \frac{1}{\sqrt{M}},$$

or $A_1 \sim ||u_x(x,0)||_2$.

PROOF: The proof is by induction on n. Precisely stated, there is a double induction hypothesis:

$$(\#1) \quad ||Du_n||_2 \le \frac{A_1}{\sqrt{M}} (1 + \sqrt{2}\, B_1 \Delta t)^n,$$

$$(\#2) \quad ||u_n||_\infty \le A_0 + B_1\, n\Delta t + \frac{1}{2} A_1 (1 + \sqrt{2}\, B_1 \Delta t)^n$$

for $0 \le n \le N$. Clearly both hypotheses hold for $n = 0,1$.

First, to prove (#1) for $||Du_{n+1}||_2$: by induction,

$$||u_{n-1}||_\infty, ||u_n||_\infty \le A_0 + B_1\, n\Delta t + \frac{1}{2} A_1 (1 + \sqrt{2}\, B_2 \Delta t)^n \quad \text{by (\#2)},$$

$$\le A_0 + B_1 T + \frac{1}{2} A_1 \exp(1 + \sqrt{2}\, B_2 T) \le A \text{ by (7.5)}.$$

An equation for Du_{n+1} follows from (7.1):

$$(I - \frac{\lambda}{2} (E - 2I + E^{-1})) (u_{n+1}^{m+1} - u_{n+1}^{m}) \tag{7.6b}$$

$$= (I + \frac{\lambda}{2} (E - 2I + E^{-1})) (u_n^{m+1} - u_n^{m})$$

$$+ \Delta t (G (u_n^{m+1}, u_{n-1}^{m+1}) - G (u_n^{m}, u_{n-1}^{m})).$$

Write

$$u_{n+1}^{m+1} - u_{n+1}^{m} = \sum_{p=0}^{M-1} \beta_{n+1}^{p} \frac{1}{\sqrt{M}} \exp (+ 2\pi i \frac{pm}{M}) \tag{7.6c}$$

$$u_n^{m+1} - u_n^{m} = \sum_{p=0}^{M-1} \beta_n^{p} \frac{1}{\sqrt{M}} \exp (+ 2\pi i \frac{pm}{M})$$

$$G(u_n^{m+1}, u_{n-1}^{m+1}) - G(u_n^{m}, u_{n-1}^{m}) = \sum_{p=0}^{M-1} \gamma^{p} \frac{1}{\sqrt{M}} \exp (+ 2\pi i \frac{pm}{M}),$$

and substitute (7.6c) into (7.6b) to obtain (using (5.6))

$$\beta_{n+1}^{p} = \frac{1 - 2\lambda (\sin \frac{p\pi}{M})^2}{1 + 2\lambda (\sin \frac{p\pi}{M})^2} \beta_n^{p} + \frac{\Delta t}{1 + 2\lambda (\sin \frac{p\pi}{M})^2} \gamma^{p}. \tag{7.6d}$$

Consequently, writing $\langle\alpha^p\rangle$ for the vector $\langle\alpha^0,\alpha^1,\alpha^2, \ldots\rangle$,

$$\left\|\langle\beta^p_{n+1}\rangle\right\|_2 \leq \left\|\left\langle\frac{1 - 2\lambda(\sin\frac{p\pi}{M})^2}{1 + 2\lambda(\sin\frac{p\pi}{M})^2}\,\beta^p_n\right\rangle\right\|_2$$

$$+ \left\|\left\langle\frac{\Delta t}{1 + 2\lambda(\sin\frac{p\pi}{M})^2}\,\gamma^p\right\rangle\right\|_2,$$

so $$\left\|\langle\beta^p_{n+1}\rangle\right\|_2 \leq \left\|\langle\beta^p_n\rangle\right\|_2 + \Delta t\left\|\langle\gamma^p\rangle\right\|_2. \tag{7.6e}$$

Since the expansions (7.6c) are norm-preserving in that

$$\sum_m \left|u^{m+1}_{n+1} - u^m_{n+1}\right|^2 = \sum_p \left|\beta^p_{n+1}\right|^2, \text{ etc.} \tag{7.6f}$$

which follows from the orthogonality mentioned in connection with (5.7), we have from (7.6e):

$$\|Du_{n+1}\|_2 \leq \|Du_n\|_2 + \Delta t\,\|\langle\gamma^p\rangle\|_2, \tag{7.6g}$$

and $$\|\langle\gamma^p\rangle\|_2 = \left(\sum_{m=0}^{M-1}\left|G(u^{m+1}_n, u^{m+1}_{n-1}) - G(u^m_n, u^m_{n-1})\right|^2\right)^{1/2}$$

$$\leq B_2\left(\|Du_n\|_2^2 + \|Du_{n-1}\|_2^2\right)^{1/2} \quad \text{by (7.2),}$$

$$\text{so } \|Du_{n+1}\|_2 \le \|Du_n\|_2 + B_2\left(\|Du_n\|_2^2 + \|Du_{n-1}\|_2^2\right)^{1/2}\Delta t$$

$$\le (1 + \sqrt{2}\, B_2\,\Delta t)\,\frac{A_1}{\sqrt{M}}\,(1 + \sqrt{2}\, B_2\,\Delta t)^n$$

using (#1).

This proves (#1) for $\|Du_{n+1}\|_2$. Now to prove (#2) for $\|u_{n+1}\|_\infty$.

Write $|u^m_{n+1}| \le |\hat{u}_{n+1}| + |u^m_{n+1} - \hat{u}_{n+1}|$, where the mean value u_{n+1} is defined in (7.3). Notice that for any k, $k = 2, 3, \ldots, n+1$,

$$\hat{u}_k = \hat{u}_{k-1} + \frac{1}{M}\sum_{m=0}^{m-1} G(u^m_{k-1}, u^m_{k-2})\,\Delta t. \tag{7.6h}$$

Using $\|u_{k-1}\|_\infty$, $\|u_{k-2}\|_\infty \le A$ and (7.2), there follows

$$|\hat{u}_k| \le |\hat{u}_{k-1}| + B_1\,\Delta t,$$

or

$$|\hat{u}_{n+1}| \le A_0 + (n+1)\,B_1\,\Delta t. \tag{7.6i}$$

Interestingly, the bound on $|u^m_{n+1} - \hat{u}_{n+1}|$ follows from the ℓ_2-bound on on Du_{n+1} alone. By Lemma 1 below, there exists a constant $C(\sim 1/2\,\sqrt{3})$ such that

$$|u^m_{n+1} - \hat{u}_{n+1}| \le C\,\sqrt{M}\,\|Du_{n+1}\|_2\,, \tag{7.6j}$$

and using (#1) for n+1 as proven above,

$$\left| u^m_{n+1} - \hat{u}_{n+1} \right| \leq C \sqrt{M} \frac{A_1}{\sqrt{M}} (1 + \sqrt{2}\, B_2 \Delta t)^{n+1} \tag{7.6k}$$

$$\leq \frac{A_1}{2} \exp \left(\sqrt{2}\, B_2 (n+1) \Delta t \right),$$

and $\quad \| u_{n+1} \|_\infty \leq A_0 + B_1 (n+1) \Delta t + \frac{1}{2} A_1 \exp \left(\sqrt{2}\, B_2 (n+1) \Delta t \right) \leq A.$

QED.

The key idea in the above proof involved relating the ℓ_2-bound on a first difference Du to an ℓ_∞-bound on u (actually, to $|u^m - \hat{u}|$). This relation, used here for finite-dimensional vector spaces, is actually based on a clever trick for proving convergence of the Fourier series of a C^1-function (Courant-Hilbert, vol. I). This proof will be given here as motivation for Lemma 1 below, the statement for finite-dimensional vector spaces.

Let f(x) be continuous and periodic on [0,1] with f'(x) L^2 on [0,1]. Let the formal Fourier series for f(x), f'(x) be, respectively,

$$\sum_{-\infty}^{+\infty} a_n \exp(+2\pi i n x), \quad \sum_{-\infty}^{+\infty} b_n \exp(+2\pi i n x). \tag{7.7a}$$

Then, for $n \neq 0$,

$$a_n = \int_0^1 f(x)\, \exp(-2\pi inx)dx = \frac{1}{2\pi in} \int_0^1 f'(x)\, \exp(-2\pi inx)dx$$

$$= \frac{1}{2\pi in}\ b_n. \tag{7.7b}$$

Now use Bessel's inequality

$$\sum_{-\infty}^{+\infty} |b_n|^2 \leq \int_0^1 |f'(x)|^2 dx. \tag{7.7c}$$

Notice

$$|f(x) - a_0| \leq \sum_{n\neq 0} |a_n| = \sum_{n\neq 0} \frac{1}{2\pi n} |b_n|$$

$$\leq \frac{1}{2\pi}\left(\sum_{n\neq 0} \frac{1}{n^2}\right)^{1/2} \left(\sum_{n\neq 0} |b_n|^2\right)^{1/2}, \tag{7.7d}$$

and using

$$a_o = \int_0^1 f(x)\, dx = \overline{f}, \text{ the mean value of } f, \tag{7.7e}$$

$$\sum_{n\neq 0} \frac{1}{n^2} = \frac{2\pi^2}{6} , \qquad (7.7f)$$

yields

$$|f(x) - \bar{f}| \leq \frac{1}{2\sqrt{3}} ||f'(x)||_2 \qquad (7.8)$$

Lemma 1 gives the finite dimensional form of this result.

<u>Lemma 1</u>. Let u be a vector with components $u^0, u^1, \ldots, u^{M-1}$; mean value $\hat{u}$ defined in (7.3); and first difference

$$Du = (u^1 - u^0, u^2, - u^1, \ldots, u^M - u^{M-1}), \; u^M = u^0.$$

Then (a) $$|u^m - \hat{u}| \leq \frac{1}{2\sqrt{M}} \left(\sum_{p=1}^{M+1} \frac{1}{(\sin \frac{p\pi}{M})^2} \right)^{1/2} ||Du||_2, \qquad (7.9)$$

(b) $$\sigma(M) = \frac{1}{2M} \left(\sum_{p=1}^{M-1} \frac{1}{(\sin \frac{p\pi}{M})^2} \right)^{1/2} \to \frac{1}{2\sqrt{3}} \text{ as } M \to +\infty.$$

<u>Proof</u>: Using (5.5), set

$$u^m = \sum_{p=0}^{M-1} \alpha^p \exp(+2\pi i \frac{pm}{M}) \frac{1}{\sqrt{M}} , \qquad (7.10a)$$

where $\alpha^p = \sum_{m=0}^{M-1} u^m z^{pm} \frac{1}{\sqrt{M}}$ where $z = \exp(-\frac{2\pi i}{M})$. (7.10b)

Folowing (7.7b), we want to apply integration by parts to the sum for α^p; this is equivalent to applying Abel's summation formula:

$$\sum_{m=0}^{M-1} (a_m b_m + s_m(b_{m+1} - b_m)) = b_M s_{M-1}, \quad s_m = a_0 + a_1 + \dots + a_m. \tag{7.10c}$$

So $$\alpha^p = -\frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} \frac{1 - (z^p)^{m+1}}{1 - z^p} (u^{m+1} - u^m) + \frac{1}{\sqrt{M}} \frac{1 - (z^p)^M}{1 - z^p} u^M,$$

if $p \neq 0$. (7.10d)

Since $u^0 = u^M$ and $z^M = 1$ and, by periodicity,

$$\sum_{m=0}^{M-1} \frac{1}{1 - z^p} (u^{m+1} - u^m) = 0, \tag{7.10e}$$

we get

$$\alpha^p = \sum_{m=0}^{M-1} \frac{z^p}{1 - z^p} (u^{m+1} - u^m) z^{pm} \frac{1}{\sqrt{M}} \tag{7.10f}$$

$$= \frac{z^p}{1 - z^p} \beta^p, \text{ where } u^{m+1} - u^m = \sum_{p=0}^{M-1} \beta^p \exp(+2\pi i \frac{pm}{M}) \frac{1}{\sqrt{M}}$$

defines β^p.

Notice (7.10f) is the analogue of (7.7b) (for $p \neq 0$).

Finally,

$$\left| u^m - \frac{\alpha^0}{\sqrt{M}} \right| = \left| \sum_{p=1}^{M-1} \alpha^p \, \bar{z}^{pm} \frac{1}{\sqrt{M}} \right| \tag{7.10g}$$

$$= \left| \sum_{p=1}^{M-1} \frac{z^p}{1 - z^p} \beta^p \, \bar{z}^{pm} \frac{1}{\sqrt{M}} \right|$$

$$\leq \frac{1}{\sqrt{M}} \left(\sum_{p=1}^{M-1} \frac{1}{|1 - z^p|^2} \right)^{1/2} \left(\sum_{p=1}^{M-1} |\beta^p|^2 \right)^{1/2} .$$

Since $|1 - z^p| = 2 \sin (\frac{p\pi}{M})$ and $\alpha^0 = \frac{1}{\sqrt{M}} \sum_{m=0}^{M-1} u^m$,

it follows that

$$|u^m - \hat{u}| \leq \frac{1}{2\sqrt{M}} \left(\sum_{p=1}^{M-1} \frac{1}{(\sin \frac{p\pi}{M})^2} \right)^{1/2} ||Du||_2, \tag{7.10h}$$

proving (7.9a).

To obtain (7.9b), note that for large M, the major contributions to the sum are for $p\pi/M$ closes to 0 and close to π, that is, for p small compared to M and p nearly equal to M. So

$$\sum_{p=1}^{M-1} \frac{1}{(\sin \frac{p\pi}{M})^2} \sim 2 \left[\frac{1}{(\pi/_M)^2} + \frac{1}{(2\pi/_M)^2} + \frac{1}{(3\pi/_M)^2} + \ldots \right]$$

$$\sim \frac{2M^2}{\pi^2} \left[1 + \frac{1}{2^2} + \frac{1}{3^2} + \ldots\right] = \frac{M^2}{3} . \tag{7.10i}$$

So $$\sigma(M) = \frac{1}{2M}\left(\sum_{p=1}^{M-1} \frac{1}{(\sin \frac{p\pi}{M})^2}\right)^{1/2} \sim \frac{1}{2\sqrt{3}} \quad \text{as } M \to \infty. \quad \text{QED.} \tag{7.10j}$$

The following values indicate how rapidly $\sigma(M) \to 1/2\sqrt{3}$:

$M = 5$	(M)	$= .28284$	(7.11)
10		.28723	
20		.28831	
30		.28851	
	$1/2\sqrt{3}$	$= .28868.$	

CHAPTER VI

TRAVELING WAVES IN REACTION-DIFFUSION SYSTEMS

INTRODUCTION

This chapter discusses periodic traveling wave solutions of

$$\underset{\sim}{u}_t = F(\underset{\sim}{u}) + K\nabla^2\underset{\sim}{u}, \tag{1.1}$$

where $\underset{\sim}{u}$ is an N-vector and K is a positive-definite matrix. The usual traveling wave substitution converts this system to a system of ordinary differential equations of order 2N. There are two natural ways for traveling waves to arise in such a system. Small amplitude waves may arise as the result of a Hopf bifurcation. This possibility was investigated by Howard and Kopell and their results are discussed in Chapter I, Section 2. Briefly, they found such small amplitude waves to exist under very general conditions, but the waves are linearly unstable. A second case arises by substitution $\xi = \sqrt{\epsilon}\,\underset{\sim}{A}\cdot\underset{\sim}{x} + \rho t$, $\underset{\sim}{A}$ = unit vector, in which case the reaction-diffusion equations become

$$\rho\underset{\sim}{u}' = F(\underset{\sim}{u}) + \epsilon K\underset{\sim}{u}'' \tag{1.2}$$

for $\underset{\sim}{u}(\xi)$. For $\epsilon = 0$ (and $\beta = 1$) the reduced system $\underset{\sim}{u}' = F(\underset{\sim}{u})$ is assumed to have a limit cycle $\underset{\sim}{U}(\xi)$ with period T. Kopell and Howard (1973) have shown that a periodic solution to (1.2) for $\epsilon \neq 0$ can be formed as a perturbation off the limit cycle solution; this solution yields large amplitude traveling waves for (1.1).

Kopell and Howard proved the *existence of periodic solutions* to (1.2) for $\epsilon \neq 0$ by an integral equation construction. The main result of this chapter is to give a second proof of this result by a series expansion. Previous work along this line has been given by Wasow (1976); the series expansions there, however, were at best asymptotic -- in particular, they were not shown to converge. The expansion constructed in this chapter will be shown to be convergent. Furthermore, it is constructed in a rather unusual way: instead of simply matching terms of $O(\epsilon^n)$, the essential factor in obtaining convergence is to mix $O(\epsilon^{n-1})$ and $O(\epsilon^n)$ terms.

The remainder of this section gives a number of related results from the literature for background and then summarizes Kopell and Howard's proof.

The second section discusses in detail the related work by Wasow on series expansions.

The third *section contains* the *main* results of this chapter: the construction of a formal expansion for periodic solutions of (1.2) when $\epsilon \neq 0$ and the proof of convergence of that expansion.

In discussing general results on the perturbation of periodic solutions, it is necessary to distinguish two basic cases: the <u>autonomous</u> and <u>nonautonomous</u> systems, respectively,

$$\underset{\sim}{v}' = F(\underset{\sim}{v}; \epsilon) \tag{1.3a}$$

$$\underset{\sim}{v}' = F(\underset{\sim}{v}, t; \epsilon) \text{ , where } F \text{ has period } T \text{ in } t. \tag{1.3b}$$

Both systems are assumed regular in ϵ and to have stable periodic solutions $\underset{\sim}{v} = \underset{\sim}{V}(t)$ with period T at $\epsilon = 0$, and the basic question is whether they continue to possess periodic solutions for $\epsilon \neq 0$. Notice that the new periodic solutions $\underset{\sim}{V}(t; \epsilon)$ for the nonautonomous case, if they exist, necessarily continue to have period T. For the autonomous systems, however, the periodic solutions $\underset{\sim}{V}(t; \epsilon)$ usually have new periods $T(\epsilon)$ with $T(0) = T$. The dependence of the period on ϵ makes the autonomous systems more awkward to work with. Although some results on the nonautonomous case will be mentioned, the autonomous case is of primary interest here. (It is also assumed that the periodic solution at $\epsilon = 0$ is nonconstant. In a Hopf bifurcation, for instance, ϵ may measure amplitude so that $\underset{\sim}{V}(t; \epsilon) \to$ constant and the period $T(\epsilon) \to T \neq 0$ as $\epsilon \to 0$.) The persistence of periodic solutions for both systems of (1.3) for $\epsilon \neq 0$ is shown in Coddington and Levinson (1955, Chapter 14).

The cases in (1.3) have "singular perturbation" counterparts:

$$\underset{\sim}{v}_1' = F_1(\underset{\sim}{v}_1, \underset{\sim}{v}_2; \epsilon) \tag{1.4A}$$

$$\epsilon \underset{\sim}{v}_2' = F_2(\underset{\sim}{v}_1, \underset{\sim}{v}_2; \epsilon) \quad ;$$

$$\underset{\sim}{v}_1' = F_1(\underset{\sim}{v}_1, \underset{\sim}{v}_2, t; \epsilon) \tag{1.4b}$$

$$\underset{\sim}{v}_2' = F_2(\underset{\sim}{v}_1, \underset{\sim}{v}_2, t; \epsilon), \quad F_1 \text{ and } F_2 \text{ have period } T \text{ in } t;$$

where again the reduced systems (formed by setting $\epsilon = 0$) are assumed to have T-period solutions $(\underset{\sim}{v}_1, \underset{\sim}{v}_2) = (\underset{\sim}{V}_1(t), \underset{\sim}{V}_2(t))$; the basic question is still the persistence of periodic solutions for $\epsilon \neq 0$. As Wasow (1976, Chapter 10) points out, no boundary layer phenomena occur in this context and the equations (1.4) should only be considered a singular perturbation problem in a formal sense.

Before discussing results for the singular case, something should be said about methods of proof. Three basic types of proofs used to show the persistence of periodic solutions for $\epsilon \neq 0$ are

(1) To show existence of a Poincaré map;

(2) To reformulate the problem as an integral equation and prove existence of solutions;

(3) To construct a series expansion and prove convergence.

A Poincaré map is a mapping from a region in phase space into itself generated by the trajectories of a system of differential equations: if the trajectories leave the region and after a finite time T enter it again, then a continuous mapping of the region into itself is generated, the Brower Fixed Point Theorem is applied, and the existence of a periodic trajectory (a trajectory meeting itself after finite time) follows.

For example, the proofs of persistence of a periodic solution for the regular cases (1.3a,b) in Coddington and Levinson (1955) are closely related to the idea of a Poincaré map, although the proofs are not expressed in such geometrical language. They construct a mapping similar to the Poincaré map such that a periodic solution will exist if the Jacobian of the mapping does not vanish; the Jacobian is shown to be nonzero at $\epsilon = 0$, and smoothness shows that it does not vanish for $\epsilon \neq 0$.

For the singular cases (1.4a,b), Flatto and Levinson (1955) prove the existence of periodic solutions for $\epsilon \neq 0$ in the nonautonomous case by reformulating the system as an integral equation. They do not consider the autonomous case directly but do remark that their results can be modified "in a familiar way" to give a proof for the autonomous case. They refer, apparently to illustrate this familiar way, to Friedrichs and Wasow (1946), who prove the existence of periodic solutions for the autonomous case (1.3a) with v_2 scalar. The Friedrichs and Wasow proof, however, is a Poincare map construction.

Wasow (1976) considers both cases (1.4a,b) in a somewhat indirect fashion so far as a definite proof of existence of periodic solutions for $\epsilon \neq 0$ is concerned. For example, in the nonautonomous case (1.3b), he sets:

$$\begin{bmatrix} \underset{\sim}{v}_1 \\ \\ \underset{\sim}{v}_2 \end{bmatrix} = \begin{bmatrix} \underset{\sim}{V}_1(t) \\ \\ \underset{\sim}{V}_2(t) \end{bmatrix} + \underset{\sim}{z} , \qquad \underset{\sim}{z} = \sum_{n=1}^{\infty} \underset{\sim}{y}_n(t)\epsilon^n ,$$

and shows that the $\underset{\sim}{y}_n$'s can be recursively solved for as periodic functions, so that a formal solution exists (Wasow, 1976, p.317). Then, instead of proving convergence of the infinite series $\underset{\sim}{z}$, he assumes the existence of an analytic periodic function $\hat{\underset{\sim}{z}}(t,\epsilon)$ which is "asymptotically represented" by the series $\underset{\sim}{z}$ as $\epsilon \to 0^+$. Setting $\underset{\sim}{z} = \hat{\underset{\sim}{z}} + \underset{\sim}{w}(t,\epsilon)$, he then proves that $\underset{\sim}{w}(t,\epsilon) \sim 0$ as $\epsilon \to 0^+$, and therefore his main result on this expansion (Theorem (45.1), p.319) is an asymptotic one:

$$\begin{bmatrix} v_1 \\ \\ v_2 \end{bmatrix} \sim \begin{bmatrix} V_1(t) \\ \\ V_2(t) \end{bmatrix} + \sum_{n=1}^{\infty} y_n(t)\epsilon^n \quad \text{as } \epsilon \to 0^+.$$

In particular, the convergence of this infinite series is not shown.

Wasow's formal expansion for the autonomous case is given in detail in the next section, and we only note here that he claims the expansion at most to be asymptotic to the true solution as $\epsilon \to 0$.

In short, the literature appears to give no general results for the persistence of periodic solutions to the autonomous case (1.4a), which explains why Kopell and Howard had to construct their own proof for the persistence of periodic solutions to (1.2).

Kopell and Howard's proof is based on rewriting the system (1.2) as an integral equation and proving convergence of an iterative solution procedure. To obtain that integral equation, they rewrite (1.2) in a very unusual way. (It should be mentioned that the results of this chapter -- the convergence proof of a series expansion in section 3 — did not result from a direct attempt to obtain such a proof. Originally, the desire was simply to understand why their unusual reformulation of the system worked at all, and as that understanding grew, its relation to a series expansion becaome clearer.)

It seems worthwhile, therefore, to discuss Kopell and Howard's approach to (1.2) in some detail before moving to series approaches in the next section. First, notice that the natural reformulation of (1.2) would be to set $\underset{\sim}{v} = \underset{\sim}{u}'$ (or $K\underset{\sim}{u}'$), obtaining:

$$\begin{aligned} \underset{\sim}{u}' &= \underset{\sim}{v} \\ \epsilon \underset{\sim}{v}' &= \beta K^{-1}\underset{\sim}{v} - K^{-1}F(\underset{\sim}{u}) . \end{aligned}$$

However, Kopell and Hward set $\underset{\sim}{v} = K\underset{\sim}{u}''$, obtaining an equation for $\underset{\sim}{v}'$ by differentiating (1.2) to get

$$\begin{aligned} \beta \underset{\sim}{u}' &= F(\underset{\sim}{u}) + \underset{\sim}{v} \\ \underset{\sim}{v}' &= \frac{\beta}{\epsilon} K^{-1}\underset{\sim}{v} - \frac{1}{\beta} F'(\underset{\sim}{u})(F(\underset{\sim}{u}) + \underset{\sim}{v}) . \end{aligned} \tag{1.5}$$

(Some minor changes in their fomulation have been made here to keep a notation consistent with (1.2).) Introducing $\underset{\sim}{u} = \underset{\sim}{U}(\xi) + \underset{\sim}{w}(\xi)$, where $\underset{\sim}{U}$ is the limit cycle, and rewriting the equations with $\beta = 1 + \hat{\beta}$ gives

$$\frac{d\underset{\sim}{v}}{d\xi} = \frac{\beta}{\epsilon}K^{-1} - \frac{1}{\beta}F(\underset{\sim}{U}+\underset{\sim}{w})\underset{\sim}{v} - \frac{1}{\beta}F'(\underset{\sim}{U}+\underset{\sim}{w})F(\underset{\sim}{U}+\underset{\sim}{w}) \tag{1.6}$$

$$\frac{d\underset{\sim}{w}}{d\xi} = F'(\underset{\sim}{U})\underset{\sim}{w} - \hat{\beta}F(\underset{\sim}{U}) + \frac{1}{\beta}\underset{\sim}{v} + R(\underset{\sim}{w},\hat{\beta},\xi) .$$

The idea is to determine β so that this sytem has a T-periodic solution. The recursive procedure can be written as

$$\underset{\sim}{v}'_n = \frac{\beta_{n-1}}{\epsilon}K^{-1} - \frac{1}{\beta_{n-1}}F'(\underset{\sim}{U}+\underset{\sim}{w}_{n-1})\underset{\sim}{v}_n - \frac{1}{\beta_{n-1}}F'(\underset{\sim}{U}+\underset{\sim}{w}_{n-1})F(\underset{\sim}{U}+\underset{\sim}{w}_{n-1})$$

$$\underset{\sim}{w}'_n = F'(\underset{\sim}{U})\underset{\sim}{w}_n - \hat{\beta}_nF(\underset{\sim}{U}) + \frac{1}{\beta_{n-1}}\underset{\sim}{v}_n + R(\underset{\sim}{w}_{n-1},\beta_{n-1},\xi). \tag{1.7a}$$

Starting with $\underset{\sim}{w}_0 = 0$, (1.7a) is solved for a T-periodic solution $\underset{\sim}{v}_1$, then (1.7b) is solved for a T-periodic solution $\underset{\sim}{w}_1$ (which determines $\hat{\beta}_1$; $\hat{\beta}_0 = 0$); then (1.7a) is solved for $\underset{\sim}{v}_2$, etc. The integral equation part of the proof comes from the fact that each step is just solving a linear, nonhomogeneous system of ODE's with the usual inversion formula (Lemma B in Appendix I).

The brilliant part of their proof is the reformulation (1.5) with the term $\frac{1}{\epsilon}K^{-1}$. At first glance, one might be tempted to say the right side of (1.5) could not lead to any bound on the iterations as $\epsilon \to 0$. Nevertheless, due to their key lemma (given here as Lemma 1 in section 3), usable bounds do in fact occur.

WASOW'S EXPANSION PROCEDURE

This section gives a detailed discussion of Wasow's series expansion (Wasow, 1976, Chapter 10) for periodic solutions of (1.2) with $\epsilon \neq 0$.

Wasow only claims the expansion to be asymptotic in ϵ . To give some idea of the essential difficulty in proving convergence of a reasonable formal expansion, we first give a quick calculation in which (1.2) is expanded in the simplest possible way. That is, set

$$\beta(\epsilon) = \sum_{n=0}^{\infty} \beta_n \epsilon^n , \qquad \underset{\sim}{u} = \sum_{n=0}^{\infty} \underset{\sim}{u}_n(\zeta)\epsilon^n , \tag{2.1}$$

and expand (1.2) using

$$F(\underset{\sim}{u}) = F(\underset{\sim}{u}_0) + \sum_{n=1}^{\infty} \left[F'(\underset{\sim}{u}_0)\underset{\sim}{u}_n + F_n(\underset{\sim}{u}_0,\underset{\sim}{u}_1,\ldots,\underset{\sim}{u}_{n-1})\right]\epsilon^n , \tag{2.2}$$

where $F'(\underset{\sim}{u}_0)$ is the Jacobian matrix of F at $\underset{\sim}{u}_0(F_1(\underset{\sim}{u}_0)=0)$. The resulting equations for $\underset{\sim}{u}_n$ are

$$\beta_0 \underset{\sim}{u}_0' = F(\underset{\sim}{u}_0) \tag{2.3a}$$

for $n \geq 1$,

$$\beta_0 \underset{\sim}{u}_n' = F'(\underset{\sim}{u}_0)\underset{\sim}{u}_n + F_n(\underset{\sim}{u}_0,\ldots,\underset{\sim}{u}_{n-1}) - \sum_{m=1}^{n} \beta_m \underset{\sim}{u}_{n-m}' + K\underset{\sim}{u}_{n-1}'' . \tag{2.3b}$$

Choosing $\beta_0 = 1$ and $\underset{\sim}{u}_0(\xi) = \underset{\sim}{U}(\xi)$, the stable limit cycle with period T, the resulting equations (2.3b) become nonhomogeneous cases of the linear variational equation of the reduced system ($\epsilon = 0$). The variational equation is assumed to have one periodic solution (namely, $\underset{\sim}{U}'(\xi)$) with the rest decaying exponentially. Then (2.3b) always has a periodic solution provided the nonhomogeneous terms satisfy a certain orthogonality relation, which determines β_n. In short, the expansion (2.1), (2.3) formally makes perfect sense. However, a problem turns up when a proof of convergence is attempted. Bounds on $\underset{\sim}{u}_n$, $\underset{\sim}{u}'_n$ can only be expressed in terms of bounds on the nonhomogeneous term in (2.3b); the nonhomogeneous term depends on $\underset{\sim}{u}''_{n-1}$; consequently, an induction procedure must obtain a bound on $\underset{\sim}{u}''_n$, and apparently we can only get such a bound by differentiating (2.3b), which leads to the need for a bound on $\underset{\sim}{u}'''_{n-1}$, etc. This infinite regress must be avoided if a convergence proof is to be constructed.

Wasow's formal expansion will now be given. Although he does not explicitly prove that it is asymptotic in ϵ to the true solution, he gives some discussion of how such a proof might be devised as based on the nonautonomous case.

For clarity, his calculations (part (a) of each numbered equation below) will be given in their original notation with their original numbering from Wasow, 1976, Chapter 10, with some minor simplifications, and the corresponding equations with the direct substitution $v = u'$ (part (b)) and the Kopell and Howard substitution $v = Ku''$ (part (c)) will be studied also. Since Wasow does not introduce a period correction immediately, we first derive the ODE form (1.1) by setting $\xi = \sqrt{\epsilon}\, \underset{\sim}{A} \cdot \underset{\sim}{x} + t$, $\underset{\sim}{A}$ = unit vector.

The original system has the form:

$$\begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix} \frac{dy}{dt} = f(y,\epsilon) \qquad (45.21)\ (2.4a)$$

$$\epsilon \frac{dv}{d\xi} = K^{-1}v - K^{-1}F(u) \qquad (\text{using } v = u') \qquad (2.4b)$$

$$\frac{du}{d\xi} = v$$

$$\epsilon \frac{dv}{d\xi} = K^{-1}v - F'(u)(F(u) + \epsilon v) \quad (\text{using } v = Ku'') \qquad (2.4c)$$

$$\frac{du}{d\xi} = F(u) + \epsilon v\ .$$

Here in (2.4a), the identity matrices I are assumed NxN and y is a $2N$-vector; u,v are N-vectors. The reduced system

$$\begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix} \frac{dy_0}{dt} = f(y_0, 0) \qquad (45.22)\ (2.5a)$$

$$0 = K^{-1}v_0 - K^{-1}F(u_0) \qquad (2.5b)$$

$$\frac{du_0}{d\xi} = v_0$$

$$0 = K^{-1}v_0 - F'(u_0)F(u_0) \qquad (2.5c)$$

$$\frac{du_0}{d\xi} = F(u_0)$$

is assumed to have a T-periodic solution $y_0(t)$ (or $U(\xi)$, $V(\xi)$), and the Jacobian matrix

$$A(t,\epsilon) = f_y(y_0,\epsilon) \qquad (2.6a)$$

$$A(\xi,\epsilon) = \begin{bmatrix} K^{-1} & -K^{-1}F'(U) \\ I & 0 \end{bmatrix} \qquad (2.6b)$$

$$A(\xi,\epsilon) = \begin{bmatrix} K^{-1} - F'(U) & -(F'F)'(U) \\ \epsilon I & F'(U) \end{bmatrix} \qquad (2.6c)$$

is to satisfy Assumption I (Wasow, p. 289, with $s = 2$), which means in this context that the first N rows and N columns of $A(t,0)$ have a nonvanishing determinant for all t-values in question (in (2.6b,c), this means K^{-1} is to be nonsingular, which it certainly is). Since the period of the perturbed solutions generally depend on ϵ, a change of variables

$$t \text{ (or } \xi) = \frac{\pi(\epsilon)}{T}\tau \qquad \textit{(45.27)}\ (2.7)$$

is made, with $\pi(\epsilon)$ to be chosen so that all solutions are to have period T with respect to τ . The new equation in τ is then

$$\begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix} \frac{dy}{dt} = \frac{\pi(\epsilon)}{T} f(y,\epsilon) \tag{2.8a}$$

$$\epsilon \frac{dv}{d\tau} = \frac{\pi(\epsilon)}{T}\left[K^{-1}v - K^{-1}F(u)\right] \tag{2.8b}$$

$$\frac{du}{d\tau} = \frac{\pi(\epsilon)}{T} v$$

$$\epsilon \frac{dv}{d\tau} = \frac{\pi(\epsilon)}{T}\left[K^{-1}v - F'(u)(F(u) + v)\right] \tag{2.8c}$$

$$\frac{du}{d\tau} = \frac{\pi(\epsilon)}{T} [F(u) + v].$$

(Incidentally, for actual computation t or $\xi = \tau/T\pi(\epsilon)$ would be better, since $\pi(\epsilon)$ would then occur on the left side of the equation, multiplying fewer terms.)

Introducing $y = y_0(\tau) + z(\tau)$ (or $(u,v) = (U(\tau) + w, V(\tau) + z)$) an equation for z (or w,z) results:

$$\begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix} \frac{dz}{d\tau} = \left\{ f(y_0,\epsilon) - f(y_0,0) - \begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix} \frac{dy_0}{d\tau} \right\} + \left(\frac{\pi(\epsilon)}{T} - 1\right) f(y_0,\epsilon)$$

$$+ \frac{\pi(\epsilon)}{T} f_y(y_0,\epsilon)z + \frac{\pi(\epsilon)}{T}\left(f(y_0+z,\epsilon) - f(y_0,\epsilon) - f_y(y_0,\epsilon)z\right)$$

$$= \epsilon\, a(\tau,\epsilon) + \left(\frac{\pi(\epsilon)}{T} - 1\right) f(y_0,\epsilon) + \frac{\pi(\epsilon)}{T} f_y(y_0,\epsilon)z + \frac{\pi(\epsilon)}{T} g(\tau,z,\epsilon)$$

(45.30) (2.9a)

$$\begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix}\begin{bmatrix} dz/d\tau \\ dw/d\tau \end{bmatrix} = \begin{bmatrix} -dz/d\tau \\ 0 \end{bmatrix} + \left(\frac{\pi(\epsilon)}{T} - 1\right)\begin{bmatrix} K^{-1}V & -K^{-1}F(U) \\ & K^{-1}V \end{bmatrix} \tag{2.9b}$$

$$+ \frac{\pi(\epsilon)}{T}\begin{bmatrix} K^{-1} & -K^{-1}F'(U) \\ I & 0 \end{bmatrix}\begin{bmatrix} z \\ w \end{bmatrix} + \frac{\pi(\epsilon)}{T}\begin{bmatrix} -K^{-1}(F(U+w)-F(U)-F'(U)w) \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix}\begin{bmatrix} dz/d\tau \\ dw/d\tau \end{bmatrix} = \begin{bmatrix} -F'(U)V \\ 0 \end{bmatrix} + \left(\frac{\pi(\epsilon)}{T} - 1\right)\begin{bmatrix} K^{-1}V-F'(U)(F(U)+\epsilon V) \\ F(U)+\epsilon V \end{bmatrix} \tag{2.9c}$$

$$+ \frac{\pi(\epsilon)}{T}\begin{bmatrix} K^{-1} - \epsilon F'(U) & -(F'F)'(U)+\epsilon\nabla F'(U) \\ \epsilon & F'(U) \end{bmatrix}\begin{bmatrix} z \\ w \end{bmatrix}$$

$$+ \frac{\pi(\epsilon)}{T}\begin{bmatrix} -F'(U+w)(F(U+w)+\epsilon(V+z))+F'(U)(F(U)+\epsilon V) \\ +F'(U)\epsilon w+(F'F)'(U)w-\epsilon\nabla\cdot F'(U)w \\ F(U+w)-F(U)-F'(U)w \end{bmatrix} .$$

Substituting

$$z(\tau) = \sum_{n=1}^{\infty} y_n(\tau)\epsilon^n \tag{2.10}$$

$$\frac{\pi(\epsilon)}{T} = 1 + \sum_{n=1}^{\infty} p_n{}^n$$

into (2.7) gives a sequence of linear equations for the y_n. The coefficient matrix for these linear systems is given by (using the notation of Assumption (B), p. 314):

$$A(\tau,0) = \begin{bmatrix} A_{110}(\tau) & A_{120}(\tau) \\ A_{210}(\tau) & A_{220}(\tau) \end{bmatrix} , \tag{2.11a}$$

$$A(\tau,0) = \begin{bmatrix} K^{-1} & -K^{-1}F'(U) \\ I & 0 \end{bmatrix} , \tag{2.11b}$$

$$A(\tau,0) = \begin{bmatrix} K^{-1} & -(F'F)'(U) \\ 0 & F'(U) \end{bmatrix} . \tag{2.11c}$$

The linear equations for the y_n are (splitting y_n into two N-vectors $y_n = (y_n^{(1)}, y_n^{(2)})$):

$$0 = A_{110}(\tau)y_n^{(1)}+A_{120}(\tau)y_n^{(2)}+\phi_n^{(1)} \tag{2.12}$$

$$\frac{dy_n^{(2)}}{d\tau} = A_{120}(\tau)y_n^{(1)}+A_{220}(\tau)y_n^{(2)}+\phi_n^{(2)}+p_n f^{(2)}(y_0(\tau),0) , \quad n = 1,2,\ldots,$$

where the ϕ_n represent preceding known terms.

Wasow notes that, assuming the homogeneous linear system has a single periodic solution, p_n is uniquely determined by the requirement of periodicity for y_n, and that a formal series solution can be generated. As to the validity of the formal series as a representation of the real solution, Wasow says (p.324);

> "It remains to show that there exists a true periodic solution z and a corresponding period $\pi(\epsilon)$ that have these series as asymptotic expansions. We shall omit these arguments. The proof can be patterned after the nonautonomous case by ... ."

Roughly speaking, the proof would be to treat (2.9) as a nonautonomous equation (containing the initially unknown function $\pi(\epsilon)$) and proceed as in the nonautonomous case. (It would be necessary to use assumption (B*) of p.322:

(a) As $\epsilon \to 0^+$, the angles of the unbounded eigenvalues of

$$\begin{bmatrix} \epsilon I & 0 \\ 0 & I \end{bmatrix} A(\tau,\epsilon) \qquad \text{do not tend to } \pm\pi/2 \;;$$

(b) The Floquet system $\frac{dx}{d\tau}\ [A_{220}(\tau)-A_{210}(\tau)A_{110}^{-1}(\tau)A_{120}(\tau)]x$ has exactly one characteristic exponent which is an integral multiple of $2\pi i$.)

As already noted, however, Wasow only claims the formal expansion for the nonautonomous case to be an asymptotic result. We conclude that once the details have been supplied for the remainder of the proof in the autonomous case, the result is only the asymptotic validity of the expansion (2.10) as $\epsilon \to 0^+$, and in particular, the convergence of the series (2.10) is not claimed.

DIRECT EXPANSION WITH PROOF FOR PERIODIC TRAVELING WAVES

This section constructs a convergent series expansion for periodic traveling waves of (1.1), thereby giving a new proof of their existence (originally shown by Kopell and Howard's iterative construction). The formal expansion is given first to motivate as much as possible assumptions and lemmas. In this section, $u, v, u_n, v_n, \ldots$ will be N-dimensional vectors with components $u = (u^{(1)}, u^{(2)}, \ldots, u^{(N)})$; $F, G, \ldots$ will be used for both vector or matrix functions. Exceptions to this rule will be obvious from context.

Substitution of $\xi = \sqrt{\epsilon}\,\underset{\sim}{A}\cdot\underset{\sim}{x} + t$, $\underset{\sim}{A}$ = unit vector, and $u = u(\xi)$ into (1.1) gives

$$\frac{du}{d\xi} = F(u) + K\frac{d^2u}{d\xi^2}, \qquad K = \text{positive-definite matrix.} \tag{3.1}$$

For $\epsilon = 0$, the system has the limit cycle solution $u = U(\xi)$ with period T. Following Kopell and Howard, we introduce $v = Ku''$ and rescale the independent variable by $\xi = \tau/\beta(\epsilon)$:

$$\beta\frac{du}{d\tau} = F(u) + \epsilon v \tag{3.2}$$

$$\epsilon\beta\frac{dv}{d\tau} = K^{-1}v - F'(u)(F(u) + \epsilon v),$$

where $\beta(\epsilon)$ is determined by requiring the solution to have period T in ξ. Expand:

$$\beta(\epsilon) = \sum_{n=0} \beta_n \epsilon^n , \tag{3.3a}$$

$$\begin{bmatrix} u \\ v \end{bmatrix} = \sum_{n=0} \begin{bmatrix} u_n \\ v_n \end{bmatrix} \epsilon^n , \tag{3.3b}$$

$$F(u) = F(u_0) + F'(u_0)(u-u_0) + \sum_{n=1} F_n(u_0,u_1,\ldots,u_{n-1})\epsilon^n, \tag{3.3c}$$

$$F'(u) = F'(u_0) + \nabla\cdot F'(u_0)(u-u_0) + \sum_{n=1} F'_n(u_0,u_1,\ldots,u_{n-1})\epsilon^n,$$

$$F'(u)F(u) = F'(u_0)F(u_0) + (F'F)'(u_0)(u-u_0) + \sum_{n=1} G_n(u_0,u_1,\ldots,u_{n-1})\epsilon^n$$

Here $u_n, v_n, F(u), F'(u)F(u)$ are N-component vectors; $F'(u)$ and $\nabla\cdot F'(u)$ are NxN matrices. Although $F_1 \equiv F'_1 \equiv G_1 \equiv 0$, these terms are retained in the expansions for notational convenience in the formal manipulations below.

The notation used in (3.3) is simpler than that of the expansions of N-component systems in Appendix II. In Appendix II, however, the expansion was in terms of the N-1 expansion parameters $E=(e_1,e_2,\ldots,e_{N-1})$, while here only one expansion parameter ϵ is used. Required properties of the terms in the expansion will only be briefly given below, since these properties have been discussed in some detail in the more general expansion of Appendix II.

Substitution of (3.3) into (3.2) gives

$$\sum_{n=0}^{\infty}\left(\sum_{m=0}^{n}\beta_{n-m}\frac{du_m}{d\tau}\right)\epsilon^n = F(u_0) + \sum_{n=1}^{\infty}[F'(u_0)u_n+F_n(u_0,u_1,\ldots,u_{n-1})]\epsilon^n$$

$$+\sum_{n=0} v_n\epsilon^{n+1} \quad ;$$

$$\sum_{n=0}^{\infty}\left(\sum_{m=0}^{n}\beta_{n-m}\frac{dv_n}{d\tau}\right)\epsilon^{n+1}=\sum_{n=0}^{\infty}(K^{-1}v_n)\epsilon^n-F'(u_0)F(u_0)$$

$$-\sum_{n=1}^{\infty}[(F'F)'(u_0)u_n+G_n(u_0,\ldots,u_{n-1})]\epsilon^n-\sum_{n=0}^{\infty}F'(u_0)v_n\epsilon^{n+1}$$

$$-\sum_{n=0}^{\infty}\left(\sum_{m=0}^{n}(\nabla\cdot F'(u_0)u_{m+1}+F'_{m+1}(u_0,\ldots,u_{m-1}))v_{n-m}\right)\epsilon^{n+2}.$$

The first of these equations yields

$$\beta_C\frac{du_0}{d\tau} = F(u_0) \tag{3.4a}$$

$$\beta_0\frac{du_n}{d\tau} = F'(u_0)u_n+F_n(u_0,u_1,\ldots,u_{n-1})+v_{n-1} - \beta_n\frac{du_0}{d\tau} - \sum_{m=1}^{n-1}\beta_n\frac{du_{n-m}}{d\tau}\ ,$$

$$n \geq 1.$$

This equation will determine u_n,β_n from preceding functions in the usual way — β_n by an orthogonality condition and u_n to be periodic. To determine v_n we mix up the terms of the second system, defining v_n by:

$$\beta_0 \frac{dv_0}{d\tau} = [\frac{1}{\epsilon} K^{-1} - F'(u_0)]v_0 - \frac{1}{\epsilon}F'(u_0)F(u_0), \tag{3.4b}$$

$$\beta_0 \frac{dv_n}{d\tau} = [\frac{1}{\epsilon} K^{-1} - F'(u_0)]v_n - \frac{1}{\epsilon}[F'F)'(u_0)u_n + G_n(u_0,\dots,u_{n-1})]$$

$$-\sum_{m=0}^{n-1} \beta_{n-m} \frac{dv_m}{d\tau} - \sum_{m=0}^{n-1} (\nabla\cdot F'(u_0)u_{m+1} + F'_{m+1}(u_0,\dots,u_m))v_{n-1-m}.$$

This equation determines v_n from u_n, β_n and preceding quantities. At first glance, it seems rather startling because of the presence of the $O(1/\epsilon)$-terms, but -- incredibly enough -- the v_n's remain $O(1)$, as shown by Lemma 2 below. This particular matching of terms is exactly the trick necessary to get a convergent series. Notice that this expansion is completely different from Wasow's expansion, as can be seen from comparing (3.4a,b) with their $O(1/\epsilon)$-terms to (2.12).

The two assumptions required for the proof are essentially the same as used in Chapter III -- existence of a stable limit cycle and analyticity:

Assumption I. The kinetic system $u'=F(u)$ has a limit cycle solution $U(\tau)$ with period T. The limit cycle is stable and the variational equation about the limit cycle has distinct characteristic exponents.

Assumption II. $F(u)$, hence $F'(u)$, $F'(u)F(u)$, are analytic at each point $u=U(\tau)$ of the limit cycle.

The first assumption says the variation equation $x'=F'(U(\tau))x$ about the limit cycle has a fundamental matrix of the form

$$X(\tau) = P(\tau)\exp(D\tau), \quad \text{where } P(\tau) \text{ is T-periodic,}$$
$$D = \mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_N) \quad \text{with } \lambda_1 = 0 \text{ and} \tag{3.5}$$
$$\mathrm{Re}(\lambda_i) \le -\mu < 0 \qquad \text{for } i = 2,\ldots,N.$$

A consequence of Assumption II is that a single majorant series applies to the totality of components of $F(u),F'(u),F'(u)F(u)$ when expanded around an arbitrary point of the limit cycle $u=U(\tau)$. That is,

there exists constant M, $R > 0$ such that (3.6)

if
(1) $f(u)$ is any component of $F(u)$, $F'(u)$, or $F'(u)F(u)$,
(2) u_0 is any point of the limit cycle $U(\tau)$,
(3) $f(u)$ is expanded about u_0 to give

$$f(u) = \sum_{n=0}^{\infty}\left(\sum_{m_1+\ldots+m_N=n} A_{m_1\ldots m_N}(u^{(1)}-u_0^{(1)})^{m_1}\ldots(u^{(N)}-u_0^{(N)})^{m_N}\right),$$

then $\left|A_{m_1\ldots m_N}\right| \le \dfrac{M}{R^n}$.

Equivalently, all choices for $f(u)$ and u_0 have a common majorant series

$$M\prod_{i=1}^{N}\left(1-\frac{u^{(i)}-u_0^{(i)}}{R}\right)^{-1} .$$

The majorant series of (3.6) enables us to obtain bounds on nonlinear terms in the recursion (3.4). Again let $f(u)$ be any component of $F(u)$, $F'(u)$, or $F'(u)F(u)$ and u_0 be any point on the limit cycle $U(\tau)$. Define functions $f_n(u_0,u_1,\ldots,u_{n-1})$ by

$$u = \sum_{n=0}^{\infty} u_n \epsilon^n , \tag{3.7a}$$

$$f(u) = f(u_0) + f'(u_0)(u-u_0) + \sum_{n=1}^{\infty} f_n(u_0,u_1,\ldots,u_{n-1})\epsilon^n.$$

(Here $f_1(u_0)\equiv 0$.) Also, for the scalar variable ζ , define

$$\zeta = \sum_{n=1}^{\infty} \zeta_n \epsilon^n , \tag{3.7b}$$

$$M(1 - \frac{\zeta}{R})^{-N} = M + \frac{MN}{R}\zeta + \sum_{n=1}^{\infty} \frac{M}{R^n} \phi_n(\zeta_1,\zeta_2,\ldots,\zeta_{n-1})^n .$$

(And $\phi_1 = 0$.) The functions f_n satisfy:

each $f_n(u_0,u_1,\ldots,u_{n-1})$ is a polynomial in the components of $u_1,\ldots,u_{n-1}$ with coefficients depending on f and u_0; (3.8a)

each f_n *satisfies the* homogeneity property

$$f_n(u_0,\alpha u_1,\alpha^2 u_2,\ldots,\alpha^{n-1} u_n) = \alpha^n f_n(u_0,u_1,\ldots,u_{n-1}) \tag{3.8b}$$

for scalar α .

Similar properties hold for the ϕ_n. From the definition of the f_n in (3.7a), the majorant series in (3.6), and the definition of ϕ_n in (3.7b), it also follows that for $|u_k| = \max_i |u_k^{(i)}|$,

$$|f_n(u_0,u_1,\ldots,u_{n-1})| \le \frac{M}{R^n} \phi_n(|u_1|, |u_2|, \ldots, |u_{n-1}|) . \quad (3.8c)$$

Therefore, if we introduce the vector norm

$$||u(\tau)|| = \sup_{1\le i\le N} \sup_{0\le\tau\le T} |u^{(i)}(\tau)| , \quad (3.9a)$$

and the compatible matrix norm

$$||A(\tau)|| = \sup_{1\le i\le N} \sup_{0\le\tau\le T} \sum_{j=1}^{N} |A_{ij}(\tau)| , \quad (3.9b)$$

then -- with f any component of $F(u)$, $F'(u)$, $F'(u)F(u)$, and u_0 any point of $U(\tau)$ -- we have

$$\sup_{0\le\tau\le T} |f_n(u_0,u_1,\ldots,u_{n-1})| \le \frac{M}{R^n} \phi_n(||u_1||, ||u_2||, \ldots, ||u_{n-1}||) \quad (3.10a)$$

Consequently, if u_0 is any point of $U(\tau)$,

$$||F_n(u_0,\ldots,u_{n-1})||, ||G_n(u_0,\ldots,u_{n-1})|| \le \frac{M}{R^n} \phi_n(||u_1||,\ldots,||u_{n-1}||) \quad (3.10b)$$

$$||F_n'(u_0,\ldots,u_{n-1})|| \le \frac{MN}{R^n} \phi_n(||u_1||, \ldots, ||u_{n-1}||) .$$

We now give two lemmas relating norms of solutions to norms of nonhomogeneous terms in the ODE's of (3.4). The first lemma is for (3.4a); the second for (3.4b).

Lemma 1. Let the matrix $A(t)$ have period T and the Floquet system $u' = A(t)u$ have a fundamental matrix $P(t)\exp(Dt)$ satisfying (3.5). Let $p_1(t)$ be the first column of $P(t)$ (that is, $p_1(t)$ is a periodic solution of $u' = Au$). Then:

(a) The equation $u' = A(t)u+b(t)+cp_1(t)$ with $b(t)$ T-periodic has a periodic solution for exactly one value of c, and for this value $|c| \le ||P^{-1}||\ ||b||$;

(b) For this value of c, a periodic solution $u(t)$ can be chosen with

$$||u|| \le (2T||P||\ ||P^{-1}||)\ ||b|| ,$$

$$||\frac{du}{d\tau}|| \le (1 + ||p_1||\ ||P^{-1}|| + 2T\,||A||\ ||P||\ ||P^{-1}||)\ ||b|| .$$

Proof: The general solution can be written as

$$u(t) = P(t)\exp(Dt)\left[a + \int_0^t \exp(-Ds)P^{-1}(s)(b(s) + cp_1(s))ds\right] .$$

Setting $P^{-1} = [q_1, q_2, \ldots, q_N]^T$, so the rows of P^{-1} are the vectors q_i^T, the integrand becomes

$$\exp(-Ds)P^{-1}(s)[b(s) + cp_1(s)] = \begin{bmatrix} q_1^T(s)b(s)+c \\ \exp(-\lambda_2 s)q_2^T b \\ \cdots \\ \exp(-\lambda_N s)q_N^T b \end{bmatrix}$$

A necessary condition for a periodic solution is that the first component be periodic, which requires

$$c = -\frac{1}{T}\int_0^T q_1^T(s)b(s)ds \; , \qquad \text{so } |c| \le ||P^{-1}|| \;\; ||b|| .$$

Applying Lemma A of Appendix I to the remaining terms gives

$$\int_0^t \exp(-\lambda_i s)q_i^T(s)b(s)ds = c^{(i)} + \exp(-\lambda_i t)r^{(i)}(t), \quad i = 2,\ldots,N,$$

where $r^{(i)}(t)$ has period T. The constants $c^{(i)}$ can be eliminated by setting $a^{(i)} = -c^{(i)}$, $i = 2,\ldots,N$. The final result is

$$u(t) = P(t) \begin{bmatrix} a^{(i)} + \int_0^t (q_i^T(s)b(s) + c)ds \\ r^{(2)}(t) \\ \cdots \\ r^{(N)}(t) \end{bmatrix}$$

Choosing $a^{(1)} = 0$, we have

$$\left|\int_0^t (q_1^T(s)b(s)+c)ds\right| \leq 2\,||P^{-1}||\ \ ||b||\ T\ ,$$

and for each $r^{(i)}(t)$,

$$|r_i(t)| \leq \left|\int_0^t \exp(\lambda_i(t-s))q_i^T(s)b(s)ds\right| \leq ||P^{-1}||\ \ ||b||\ T,$$

since $Re(\lambda_i) \leq 0$. So

$$||u|| \leq 2T\,||P||\ \ ||P^{-1}||\ \ ||b||\ ,$$

and from the equation itself

$$\left|\left|\frac{du}{dt}\right|\right| \leq [\,||A||\ (2T\,||P||\ \ ||P^{-1}||\,) + 1 + ||p_1||\ \ ||P^{-1}||\,]\,||b||.$$

Q.E.D.

Lemma 2. (Kopell and Howard, 1973)

(a) If $A(t),b(t)$ are T-periodic and $d||A||_2 \leq 1/2$, where d = largest eigenvalue of the positive-definite matrix K, then

$$\frac{du}{dt} = (\frac{1}{\epsilon}K^{-1} + A(t))u + b(t)$$

has a unique T-periodic (nontrivial) solution $u(t)$, and $||u||_2 \leq 2\epsilon d\,||b||_2$.

(b) $||u|| \leq 2\sqrt{N}\, d\, \epsilon\, ||b||$;

$||du/dt|| \leq (1 + 2\sqrt{N}\, d\, ||K^{-1}+\epsilon A(t)||)\, ||b||$.

Proof: (a) is simply a restatement of Kopell and Howard's lemma for functions with period T instead of 2π. (Incidentally, Kopell and Howard did not explicitly show existence of a periodic solution in their proof, only that if one existed, then it was unique. However, existence is an immediate consequence of their construction for the solution and the condition on ϵ.) Since their results are in terms of the Euclidean norm $|| \; ||_2$, (b) is a simple restatement of the results in the norm (3.9), using the identity

$$||u|| \leq ||u||_2 \leq \sqrt{N}\, ||u||$$

for N-dimensional vectors.

We now proceed with the proof, assuming that ϵ is sufficiently small that $\epsilon d ||F'(U(\tau))|| \leq 1/2$ holds in order to apply Lemma 2 when needed. Equations (3.4a,b) will be solved recursively for T-periodic functions u_n, v_n while determining β_n by an orthogonality condition and simultaneously constructing a majorant series for $|\beta_n|$, $||u_n||$, $||v_n||$.

From (3.4a) we have

$$\beta_0 = 1 , \qquad u_0 = U(\tau) . \tag{3.11}$$

The equation for v_0 in (3.4b) becomes

$$\frac{dv_0}{d\tau} = \left[\frac{1}{\epsilon} K^{-1} - F'(U(\tau))\right] v_0 - \frac{1}{\epsilon} U''(\tau) ,$$

and applying Lemma 2 gives a unique T-periodic solution $v_0(\tau)$ with

$$||v_0|| \leq 2d\sqrt{N}\,||U''|| , \tag{3.12}$$

$$\left|\left|\frac{dv_0}{d\tau}\right|\right| \leq \left(1 + 2d\sqrt{N}\,||K^{-1} + \epsilon F'(U(\tau))||\right) \frac{1}{\epsilon}\,||U''|| .$$

Returning to (3.4a) with $n \geq 1$, we assume β_i, u_i, v_i, $i=0,1,..,n-1$, to have been appropriately determined. Applying Lemma 1, there is a unique value of β_n determining a periodic solution $u_n(\tau)$, and u_n can be chosen to satisfy:

$$|\beta_n| \leq ||P^{-1}|| \left\{||F_n(u_0,u_1,\ldots,u_{n-1})|| + ||v_{n-1}|| + \sum_{m=1}^{n-1}|\beta_m| \left|\left|\frac{du_{n-m}}{d\tau}\right|\right|\right\} \tag{3.13a}$$

$$||u_n|| \leq 2T\,||P||\;||P^{-1}|| \quad \left\{ \text{ditto} \right\}$$

$$\left|\left|\frac{du_n}{d\tau}\right|\right| \leq \left(1 + ||P_1||\;||P^{-1}|| + 2T\,||F'(U)||\;||P||\;||P^{-1}||\right)\left\{\text{ditto}\right\}$$

From (3.4b) and Lemma 2, we have

$$\|v_n\| \le 2\sqrt{N}\,d\epsilon\left[\sum_{m=0}^{n-1}|\beta_{n-m}|\ \left\|\frac{dv_m}{d\tau}\right\| + \frac{1}{\epsilon}\left\|(F'F)'(U)u_n + G_n(u_0,\ldots,{}_{n-1})\right\|\right.$$

$$\left. + \sum_{m=0}^{n-1}\left\|\nabla\cdot F'(U)u_{m+1} + F'_{m+1}(u_0,\ldots,u_m)v_{n-1-m}\right\|\right]$$

$$\left\|\frac{dv_n}{d\tau}\right\| \le \left(1 + 2\sqrt{N}\,d\,\|K^{-1} + \epsilon F'(U)\|\right)\left[\text{ditto}\right] . \tag{3.13b}$$

Now to construct the majorant series. Pick a bound M such that

$$\|P^{-1}\|, \left(1 + \|p_1\|\ \|P^{-1}\| + 2T\,\|F'(U)\|\ \|P\|\ \|P^{-1}\|\right), 2\sqrt{N}\,d,$$

$$1 + 2\sqrt{N}\,d\,\|K^{-1} + \epsilon F'(U)\|, \|\nabla\cdot F'(U)\|, \|(F'F)'(U)\| \le \hat{M}. \tag{3.14}$$

Assume that constants U_i, V_i, $i=0,1,\ldots,n-1$, have been constructed with $|\beta_i|$, $\|u_i\|$, $\|du_i/d\tau\| \le U_i$ and $\|v_i\|$, $\|dv_i/d\tau\| \le V_i$. Notice U_0, V_0 are easily chosen from (3.11) and (3.12) (and without loss of generality we can assume $U_0, V_0 \le \hat{M}$). For $n \ge 1$, define

$$U_n = \hat{M}\left[\frac{M}{R^n}\phi_n(U_1,\ldots,U_{n-1}) + V_{n-1} + \sum_{m=1}^{n-1} U_m U_{n-m}\right]$$

$$V_n = \epsilon\hat{M}\left[\sum_{m=0}^{n-1} U_{n-m}V_m \frac{1}{\epsilon} + \left[\hat{M}U_n + \frac{M}{R^n}\phi_n(U_1,\dots,U_{n-1})\right]\frac{1}{\epsilon} + \hat{M}(U_1+\dots+U_n) + \sum_{m=0}^{n-1}\frac{NM}{R^{m+1}}\phi_{m+1}(U_1,\dots,U_m)V_{n-1-m}\right] . \qquad (3.15b)$$

From (3.10b), (3.13a), and (3.15a), it follows that $|\beta_n|$, $||u_n||$, $||du_n/d\tau|| \le U_N$. From (3.10b), (3.13b), and (3.15b), it follows that $||v_n||$, $||dv_n/d\tau|| \le V_n$.

To show convergence of the series (3.3), it is only necessary to show convergence of the majorant series

$$\hat{U}(\epsilon) = \sum_{n=1}^{\infty} \epsilon^{n-1}U_n , \qquad \hat{V}(\epsilon) = \sum_{n=1}^{\infty} {}^{n-1}V_n , \qquad (3.16)$$

for ϵ sufficiently small. Multiplying the equations of (3.15) by ϵ^{n-1}, $n \ge 1$, notice that:

$$\sum_{n=1}^{\infty} \frac{1}{R^n}\phi_n(U_1,\dots,U_{n-1})\epsilon^{n-1} = \frac{1}{\epsilon}\left[\left(1-\frac{\hat{U}}{R}\right)^{-N} - 1 - N\frac{\epsilon\hat{U}}{R}\right] \qquad (3.17)$$

$$\sum_{n=1}^{\infty}\left(\sum_{m=1}^{n-1} U_m U_{n-m}\right)\epsilon^{n-1} = \epsilon(\hat{U})^2 ,$$

$$\sum_{n=1}^{\infty}\left(\sum_{m=0}^{n-1} U_{n-m}V_m\right)\epsilon^{n-1} = \hat{U}(V_0 + \epsilon\hat{V}) ,$$

$$\sum_{n=1}^{\infty}\left(\sum_{m=1}^{n} U_m\right)\epsilon^{n-1} = \frac{1}{1-\epsilon}\hat{U} ,$$

$$\sum_{n=1}^{\infty}\left(\sum_{m=1}^{n} \frac{1}{R^m}\phi_m(U_{.},\ldots,U_{m-1})V_{n-m}\right)\epsilon^{n-1} = \frac{1}{\epsilon}(V_0+\epsilon\hat{V})\left[\left(1-\frac{\epsilon\hat{U}}{R}\right)^{-N}-1-N\frac{\epsilon\hat{U}}{R}\right]$$

From (3.15), (3.16), (3.17), we have a set of equation relating $\hat{U},\hat{V},\epsilon$:

$$\hat{U} = \frac{\hat{M}M}{\epsilon}\left[\left(1-\frac{\epsilon\hat{U}}{R}\right)^{-N}-1-N\frac{\epsilon\hat{U}}{R}\right] + \hat{M}(V_0+\epsilon\hat{V}) + \hat{M}\epsilon\hat{U}^2 \tag{3.18}$$

$$\hat{V} = \hat{M}\hat{U}(V_0+\epsilon\hat{V}) + \hat{M}^2\hat{U} + \hat{M}M\frac{1}{\epsilon}\left[\left(1-\frac{\epsilon\hat{U}}{R}\right)^{-N}-1-N\frac{\epsilon\hat{U}}{R}\right]$$

$$+\frac{\hat{M}^2\epsilon}{1-\epsilon}\hat{U} + NM\hat{M}(V_0+\epsilon\hat{V})\left[\left(1-\frac{\epsilon\hat{U}}{R}\right)^{-N}-1-N\frac{\epsilon\hat{U}}{R}\right] .$$

These two equations have the form

$$P(\hat{U},\hat{V},\epsilon) = \hat{U} - \hat{M}V_0 + O(\epsilon) = 0$$

$$Q(\hat{U},\hat{V},\epsilon) = -\hat{M}(V_0 + \hat{M})\hat{U} + \hat{V} + O(\epsilon) = 0 .$$

Since P,Q are analytic functions of U,V, at $\hat{M}V_0,\hat{M}^2V_0(V_0+\hat{M}),0$ and since the Jacobian of P,Q with respect to U,V does not vanish at this point, then the Implicit Function Theorem for complex functions gives that analytic functions $\hat{U}(\epsilon)$, $\hat{V}(\epsilon)$ exist around $\epsilon = 0$. That is, the majorants (3.16) converge for ϵ sufficiently small.

APPENDIX I

LEMMAS A, B, C, AND D

The following four lemmas are used repeatedly throughout this thesis, and it is useful to collect them in one place for easy reference. Their frequent use also suggests giving them special names - A, B, C, D - distinct from the numbering system employed in this thesis.

The first lemma is basically concerned with the result of integrating an exponential against a periodic function.

<u>LEMMA A</u>. Let $f(t)$ be C^1, periodic with period T and with mean value

$$\bar{f} = \frac{1}{T}\int_0^T f(t)dt;$$

define

$$F(t) = \int_0^t \exp(\beta s)f(s)ds, \quad \beta \text{ complex.}$$

Then (n = integer):

(1) if $\beta = \frac{2\pi i n}{T}$, then $F(t) = ct + g(t)$, where g has period T and c is a constant;

(2) if $\beta \neq \frac{2\pi i n}{T}$, then

(a) $F(t) = \exp(\beta t)g(t)-g(0)$, where $g(t)$ has period T and $\bar{g} = \frac{1}{\beta}\bar{f}$;

(b) $g(0) = \frac{1}{\exp(\beta T)-1}\int_0^T \exp(\beta s)f(s)ds$;

(c) $\sup_{[0,T]}|g(t)| \leq \left[\frac{1}{T}\int_0^T |f(s)|^2 ds\right]^{1/2}\left[\sum_{-\infty}^{+\infty}\frac{1}{(\mathrm{Re}\,\beta)^2 + \left(\frac{2\pi n}{T} - \mathrm{Im}\,\beta\right)^2}\right]^{1/2}$;

(3) if $\beta \neq \frac{2\pi i n}{T}$, then $x' + \beta x = f(t)$ has a unique T-periodic solution and it is given by $g(t)$ as defined in (2);

(4) if β is real, $f(t) \geq 0$, and $f(t) \neq 0$ for some t, then in (2), $\beta < 0$ (>0) implies $g(t) < 0$ (>0) for all t.

PROOF:

(1) Immediate.

(2) Integrate the (absolutely convergent) Fourier series termwise:

$$F(t) = \sum_{-\infty}^{+\infty} \int_0^t \exp(\beta s) a_n \exp\left(-\frac{2\pi i n s}{T}\right) ds$$

$$= \sum_{-\infty}^{+\infty} \frac{a_n}{\beta - \frac{2\pi i n}{T}} \left[\exp\left(\left(\beta - \frac{2\pi i n}{T}\right) t\right) - 1\right]$$

$$= \exp(\beta t)\left[\sum_{-\infty}^{+\infty} \frac{a_n}{\beta - \frac{2\pi i n}{T}} \exp\left(-\frac{2\pi i n}{T} t\right)\right] - g(0).$$

Existence of $g(t)$ and $\bar{g} = \frac{1}{\beta}\bar{f}$ follow from this formula.
(2c) follows from

$$|g(t)| \leq \sum \left| a_n \frac{1}{\beta - \frac{2\pi i n}{T}} \right| \leq \left(\sum |a_n|^2\right)^{1/2} \left(\sum \frac{1}{\left|\beta - \frac{2\pi i n}{T}\right|^2}\right)^{1/2}$$

and Parseval's Theorem. (2b) follows from $\exp(\beta T)g(T)-g(0)=F(T)$ and noting $g(T)=g(0)$.

(3) By direct calculation.

(4) If $\beta < 0$, notice $F(0) = 0$ and F increases to $F(+\infty) =$ positive number $= -g(0)$. So $g(0) < 0$. If $g(t_0) = 0$ for

some $t_0 > 0$, then $F(t_0) = -g(0)$, so $F(t) = -g(0)$ for $t \geq t_0$, forcing the periodic $g(t) = 0$, contradicting $g(0) < 0$. So $g(t) < 0$ for all t. Similarly for $\beta > 0$, using $t \to -\infty$. QED.

In practice, some awkwardness can occur in explicit numerical calculation of the periodic function $g(t)$ from $f(t)$ in Lemma A.2. Here,

$$g(t) = \exp(-\beta t)\left[C + \int_0^t \exp(\beta s)\ f(s)ds\right], \tag{1}$$

where $f(t)$ will be a T-periodic function, usually known only in tabulated form from other numerical work, and $C = g(0)$ is found without difficulty from Lemma A.2b.

Equation (1) as it stands involves multiplying exponen.:ally large and exponentially small quantities in t, and as the numerical integration is carried out over one period $[0,T]$, serious errors can arise even for moderate values of $|\beta T|$, say $|\beta T| \sim 20$. If $\beta > 0$, then a stepwise integration based on

$$g(t) = C\exp(-\beta t) + \int_0^t \exp(\beta(s-t))f(s)ds \tag{2}$$

works well; but if $\beta < 0$ — which is typically the case in almost all calculations of this sort in the thesis -- this expression is the difference of two exponentially growing quantities as t increases and again large errors occur.

For $\rho < 0$, these difficulties are overcome by backwards integration (which is possible because periodicit·· means $g(t)$ on $[-T,0]$ gives $g(t)$ on $[0,T]$): specifically, set $g_n = g(-nh)$ for some step size $h = T/N$ and use

$$g_0 = C,$$

$$g_n = \exp(\rho h)g_{n-1} - \int_{(n-1)h}^{nh} \exp\Big(\rho(nh-s)\Big) f(-s)ds, \qquad (3)$$

evaluating the integral by any desired scheme (in fact, in Chapter III, an extrapolation scheme -- for which periodicity is essential -- is used to give high accuracy and high efficiency in the repeated calculation of integrals of the form (1)).

For reference, the standard result on solving a non-homogeneous system of linear differential equations in terms of the homogeneous solutions is given, as well as associated results of particular use in this thesis.

LEMMA B.

(1) Let $X(t)$ be the fundamental matrix for the system of differential equations $x' = A(t)x$. Then $y' = A(t)y + b(t)$ has the general solution

$$y = X(t)\left(C + \int_{t_0}^{t} X^{-1}(s)b(s)ds\right),$$

C an arbitrary constant vector.

(2) (Abel's Identity) Let $X(t)$ be the fundamental matrix for $x' = A(t)x$ and $W(t) = \det(X(t))$. Then

$$W(t) = W(t_0)\exp\left(\int_{t_0}^{t} \mathrm{Tr}(A(s))ds\right).$$

(3) (Floquet's Theorem) Let $A(t)$ be T-periodic for the system of differential equations $x' = A(t)x$. Then the fundamental matrix can be written in the form

$$X(t) = P(t)\exp(tB),$$

where $P(t)$ has period T and B is a constant (possibly complex) matrix.

PROOF: (1), (2), and (3) are all standard results; see Coddington and Levinson (1955, Chapter 3) or Lefschetz (1977, Chapter 3). Q.E.D.

Notice that if B is reduced to Jordan canonical form by $J = C^{-1}BC$, then $X(t) = P(t)\exp(tB)$ can be rewritten as

$$X(t)C = P(t)C\exp(tJ),$$

giving a fundamental matrix as a periodic matrix multiplied by an especially simple exponential matrix.

Floquet's Theorem arises in discussing the kinetic system (I.1.2), which is assumed to possess a stable limit cycle with period T. The variational equation about the limit cycle is a Floquet system

$$\underset{\sim}{w}' = F'(\underset{\sim}{U}(t))\underset{\sim}{w} ; \tag{4}$$

notice that $\underset{\sim}{U}'(t)$ is always a solution, and the assumption of stability means all other solutions of (4) decay exponentially. Equivalently, the <u>Floquet exponents</u> (eigenvalues of the matrix B in Lemma B.2) include 0 once and the other exponents all have negative real part.

The N-component system (4) occurs in Chapters III and VI; most work is done on the two-component form of (4). In this case, the standard notation will be that of the kinetic equations of the two-component system (I.2.1), namely,

$$\begin{aligned} u' &= F(u,v) \\ v' &= G(u,v), \end{aligned} \tag{5}$$

which are assumed to possess a stable limit cycle $U(t)$, $V(t)$ with period T. In this case the variational equation about the limit cycle is the Floquet system

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} F_u(U(t),V(t)) & F_v(U(t),V(t)) \\ G_u(U(t),V(t)) & G_v(U(t),V(t)) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \tag{6}$$

which immediately has the periodic solution $(x,y) = (U'(t),V'(t))$ and, by the assumption of stability, an exponentially decaying solution. For computational purposes these results are summarized in precise form:

LEMMA C. The system (6) has a fundamental matrix

(1) $$\begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U}(t) \\ V'(t) & \exp(-\mu t)\hat{V}(t) \end{bmatrix},$$

where U',V' is the derivative of the limit cycle and U',V', $\hat{U},\hat{V}$ are real, T-periodic functions;

(2) $$-\mu = \frac{1}{T}\int_0^T (F_1(s) + G_2(s))ds \; ;$$

(3) $$\begin{bmatrix} \hat{U}(t) \\ \hat{V}(t) \end{bmatrix} = A(t)\begin{bmatrix} -V'(t) \\ U'(t) \end{bmatrix} + B(t)\begin{bmatrix} U'(t) \\ V'(t) \end{bmatrix},$$

where $A(t)$ is a T-periodic function determined (up to multiplication by a constant) by

$$(4)\qquad A(t)\left[(U'(t))^2+(V'(t))^2\right] = A(0)\left[(U'(0))^2+(V'(0))^2\right] \exp\left(\int_0^t (F_1(s) + G_2(s) + \mu)ds\right) ,$$

and $B(t)$ is the unique T-periodic solution to

$$(5)\qquad B'-\mu B = \frac{A(t)}{[(U'(t))^2+(V'(t))^2]^2}\left[(G_1+F_2)((U')^2-(V')^2)+2(G_2-F_1)U'V'\right] .$$

PROOF:

(1) U',V' is immediately a solution and the second solution has the form of an exponential multiplying a periodic function by Floquet's Theorem.

(2) Follows directly from Abel's Identity.

(3) The periodic part of the second solution is decomposed into a sum of periodic vector functions tangent to and normal to the limit cycle, a useful formulation taken from Halanay (1966, Chapter 3).

(4),(5) These follow by direct substitution of (3) into equation (6), separating components, and using the fact that $A(t)$ and $B(t)$ must have period T. Q.E.D.

In the above Lemma, the Floquet exponents of the system are 0 and $-\mu$, and $\mu > 0$ must occur because the limit cycle is assumed stable. Diliberto (1950) has made the solvability (reduction to a quadrature) of the variational equation of a two-component system the basis of several stability results on trajectories, and Lemma C appears in his work in the form of the solutions of the variational equation about an arbitrary trajectory, while here the trajectory is taken to be a limit cycle.

The important point of Lemma C is that once the stable limit cycle -- one of the easiest objects to compute numerically -- is found, all solutions of the variational equation can be found either directly or by a simple quadrature. The most awkward function, perhaps, is $B(t)$ in Lemma C.5, which would be calculated as the periodic solution given by Lemma A.3.

The preceding Lemma calculates the solution of the variational equation; the following Lemma gives information in solving the nonhomogeneous variational equation, which will occur repeatedly in various series expansions about the limit cycle.

We consider the following general nonhomogeneous equation:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} F_1(t) & F_2(t) \\ G_1(t) & G_2(t) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} b_1(t) \\ b_2(t) \end{bmatrix} + A \begin{bmatrix} U'(t) \\ V'(t) \end{bmatrix} . \tag{7}$$

LEMMA D:

(1) If $A = 0$ in (7), then the general solution is

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U}(t) \\ V'(t) & \exp(-\mu t)\hat{V}(t) \end{bmatrix}$$

$$\left\{ \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} + \int_{t_0}^{t} \begin{bmatrix} \hat{V}(s) & -\hat{U}(s) \\ -\exp(\mu s)V'(s) & \exp(\mu s)U'(s) \end{bmatrix} \begin{bmatrix} b_1(s) \\ b_2(s) \end{bmatrix} \frac{ds}{U'\hat{V}-V'\hat{U}} \right\}.$$

(2) If $b_1(t), b_2(t)$ are T-periodic in (7), then there is a unique value of A such that a T-periodic solution exists. This T-periodic solution $(x(t),y(t))$ is unique up to an additive multiple of $(U'(t),V'(t))$ (i.e., (x,y) is a solution implies $(x+aU', y+aV')$ is also a T-periodic solution for arbitrary constant a).

PROOF:

(1) Is simply Lemma B.1 applied to (7) and using the fundamental matrix of Lemma C.1. The results in (2) follow by direct calculation, given here for reference. First, the general solution (using $t_0 = 0$) is

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} U'(t) & \exp(-\mu t)\hat{U} \\ V'(t) & \exp(-\mu t)\hat{V} \end{bmatrix} \tag{8}$$

$$\left(\begin{bmatrix} C_1 \\ C_2 \end{bmatrix} + \int_{0}^{t} \begin{bmatrix} \hat{V}(s) & -\hat{U}(s) \\ -\exp(\mu s)V'(s) & \exp(\mu s)U'(s) \end{bmatrix} \begin{bmatrix} b_1(s)+AU'(s) \\ b_2(s)+AV'(s) \end{bmatrix} \frac{ds}{U'\hat{V}-V'\hat{U}} \right)$$

Using Lemma A, define

$$\int_0^t \left(\frac{\hat{V}b_1-\hat{U}b_2}{U'\hat{V}-V'\hat{U}}\right) ds = h_1 t + h(t) \quad , \tag{9a}$$

$$\int_0^t \exp(\mu s) \frac{-b_1 V'+b_2 U'}{U'\hat{V}-V'\hat{U}} ds = -k(0) + \exp(\mu t)k(t), \tag{9b}$$

where h_1, $h(t)$, $k(t)$ are uniquely determined and T-periodic.

Equation (8) then becomes:

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} U'(t) \\ V'(t) \end{bmatrix} (C_1 + At + h_1 t + h(t)) + \begin{bmatrix} \hat{U}(t) \\ \hat{V}(t) \end{bmatrix} ((C_2 - k(0))\exp(-\mu t) + k(t)).$$

Consequently, to obtain a T-periodic solution, it is necessary to choose (using Lemma A)

$$A = -h_1 = -\frac{1}{T}\int_0^T \frac{b_1\hat{V}-b_2\hat{U}}{U'\hat{V}-V'\hat{U}} ds \quad . \tag{10a}$$

$$C_2 = k(0) = \frac{1}{\exp(\mu T)-1} \int_0^T \exp(\mu s) \frac{b_2 U'-b_1 V'}{U'\hat{V}-V'\hat{U}} ds \; . \tag{10b}$$

The T-periodic solution is then

$$\begin{bmatrix} \hat{x} \\ \hat{y} \end{bmatrix} = (C_1 + h(t)) \begin{bmatrix} U'(t) \\ V'(t) \end{bmatrix} + k(t) \begin{bmatrix} \hat{U}(t) \\ \hat{V}(t) \end{bmatrix} \quad . \qquad \text{Q.E.D.}$$

NOTE: One way of uniquely specifying $(\hat{x},\hat{y})$ would be to require

$$\int_0^T (\hat{x}(s)U'(s) + \hat{y}(s)V'(s))ds = 0 , \tag{11}$$

which clearly determines C_1 uniquely.

APPENDIX II

THE EXPANSION AND PROOF OF CONVERGENCE IN THE GENERAL CASE FOR CHAPTER III

This section discusses the general case of (III.1.1), constructing the expansion and proving its convergence. For clarity, the construction is made exactly analogous to the two-component case of the second section of Chapter III, equations (4)-(7) corresponding to (III.2.1)-(III.2.4) and (8)-(13) to (III.2.6)-(III.2.11). Unfortunately, however, the proof requires the use of power series in several variables, with the consequent notational mess. This section will, therefore, begin with a discussion of notation and certain required series manipulations.

Small letters $a, u, u_1, \ldots$ are used for scalar constants and functions; capital letters $U, E, \ldots$ for vectors and matrices. Vector components are indicated by lowering the case of the letter and use of subscripts: $U = (u_1, u_2, \ldots, u_N)$, $E = (e_1, e_2, \ldots, e_{N-1}), \ldots$. Matrix components use subscripts and superscripts: P has p_i^j in its i^{th} row, j^{th} column. (So the subscript convention for vectors is consistent with column vectors.)

Small Greek letters, $\alpha, \beta, \ldots$ are used for vectors with non-negative integer components; the components are written with subscripts: $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_M)$. Associated with such vectors are:

$$|\alpha| = \sum_i \alpha_i ,$$

$$\alpha + \beta = (\alpha_1 + \beta_1, \alpha_2 + \beta_2, \ldots) , \tag{1a}$$

$$\alpha \leq \beta \text{ iff } \alpha_i < \beta_i \quad \text{for each } i,$$

$$X^\alpha = x_1^{1} x_2^{2} \ldots x_M^{M} .$$

In the monomial X^α, it is always understood that X and α have the same number of components. Notice:

$$X^\alpha X^\beta = X^{\alpha+\beta}, \tag{1b}$$

$$\left(\sum_{n=0}^{\infty} \sum_{|\alpha|=n} u(\alpha) X^\alpha\right)\left(\sum_{n=0}^{\infty} \sum_{|\beta|=n} v(\beta) X^\beta\right) = \sum_{n=0}^{\infty} \sum_{|\gamma|=n} \left(\sum_{\alpha+\beta=\gamma} u(\alpha)v(\beta)\right) X^\gamma .$$

The occasional exception to these rules will be explicitly noted.

It will be necessary to form composites of power series, as in the derivation of (III.2.5). Let $f(U) = f(u_1, u_2, \ldots, u_N)$ be a scalar function of the vector U, with f analytic. Set $E = (e_1, e_2, \ldots, e_M)$ and:

$$U = \sum_{n=0}^{\infty} \sum_{|\alpha|=n} U(\alpha) E^\alpha , \tag{2}$$

where $U(\alpha)$ are vector coefficients of the monomials E^α. Substitution of (2) into $f(U)$ gives the analogue of (III.2.5):

$$f(U) = f(U(\hat{0})) + \sum_{|\alpha|=1} \nabla f(U(\hat{0})) \cdot U(\alpha)\, E^{\alpha} \tag{3a}$$

$$+ \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \left[\nabla f(U(\hat{0})) \cdot U(\alpha) + f_{\alpha}(U(\beta):\ \beta<\alpha)\right] E^{\alpha}\ ,^{1}$$

(Homogeneity Property) given $K = (k_1, k_2, \ldots, k_M)$, then:

$$f_{\alpha}(K^{\beta} U(\beta):\ \beta<\alpha) = K^{\alpha} f_{\alpha}(U(\beta):\ \beta<\alpha). \tag{3b}$$

Here $\hat{0} = (0,0,\ldots,0)$ (M components). The term $f_{\alpha}(U(\beta):\beta<\alpha)$ is a scalar function of the N-component vectors $U(\beta)$ for $\beta<\alpha$;

$$\nabla f(U(\hat{0})) = \left[\frac{\partial f}{\partial u_1}(U(\hat{0})),\ \ldots,\ \frac{\partial f}{\partial u_N}(U(\hat{0}))\right] .$$

We shall actually substitute the series (2) into a vector function $F(U)$. For such a case, the properties (3) apply to the scalar components $F_i(U)$ individually.

The formal construction is patterned exactly on that of the third section of Chapter III. The N-component system is

$$U' = F(U) \tag{4}$$

with limit cycle $Q(t)$ with period T(scalar), $Q(0)$ specified. The variational equation about the limit cycle is the Floquet system:

$$W' = \nabla F(Q(t))W \tag{5}$$

---

[1] The terms f_{α} should be considered as defined by this equation; they are the analogues of the functions F_n in (III.2.5).

where ∇F is the matrix of first partial derivatives of the vector function F. The fundamental matrix is assumed to have the form:

$$P(t)\exp(-Dt)\ , \tag{6}$$

where $P(t)$ is a T-periodic matrix, with $Q'(t)$ in the first column and

$$D = \mathrm{diag}(0, \mu_1, \mu_2, \ldots, \mu_{N-1}) \text{ with } \mathrm{Re}(\mu_i) > 0\ .$$

It is always possible to write the characteristic matrix as $P(t)\exp(Dt)$ with $P(t)$ periodic and D in Jordan canonical form; however, the real content of (6) is the assumption that the canonical form of D be diagonal. The importance of this assumption is that solutions of (5) can be written as products of exponentials and periodic functions (so that Lemma A applies) rather than exponentials, periodic functions, and polynomials.

Introducing the expansion parameters $E=(e_1,e_2,\ldots,e_{N-1})$, a series expansion:

$$U(t) = \sum_{n=0}^{\infty} \sum_{|\alpha|=n} U(\alpha;\ t)\ E^{\alpha} \tag{7}$$

is assumed and substituted into (4). The resulting equations for $U(\alpha;t)$ (using the notation of (3) are (ϕ is scalar and $\alpha^1 = (1,0,\ldots,0)$, $\alpha^2 = (0,1,0,\ldots,0)$, etc.):

$$U'(\hat{0};t) = F(U(\hat{0};t)) \text{ with solution } U(0;t) = Q(t+\phi); \tag{8a}$$

AD-A087 114 CENTER FOR NAVAL ANALYSES ALEXANDRIA VA OPERATIONS EV--ETC F/G 7/4
LIMIT CYCLE SOLUTIONS OF REACTION-DIFFUSION EQUATIONS.(U)
JUN 80 D COPE
UNCLASSIFIED OEG-PP-287 NL

4 OF 4
AD A
087114

END
DATE
FILMED
9-80
DTIC

$$U'(\alpha^i;\ t) = \nabla F(Q(t+\phi))U(\alpha^i;\ t), \quad i = 1,2,\ldots,N-1; \tag{8b}$$

$$U'(\alpha;\ t) = \nabla F(Q(t+\phi))U(\alpha\ ;\ t) + F_\alpha(U(\beta;\ t);\ \beta < \alpha), \ |\alpha| \geq 2. \tag{8c}$$

The idea is to pick the limit cycle as the first term, as has been done, and then require all subsequent solutions to decay exponentially. Consequently, we pick the N-1 functions $U(\alpha^i;t)$ to be the N-1 exponentially decaying solutions in (6):

$$U(\alpha^i;\ t) = P^i(t)\exp(-\mu_i t)\ , \qquad i = 1,\ldots,N-1. \tag{9}$$

(The columns of $P(t)$ in (6) are $P^i(t)$, $i = 0,1,\ldots,N-1$.)

We now show that all terms $U(\alpha;t)$ in the expansion can be written in the form

$$U(\alpha;\ t) = \exp(-\alpha\cdot\mu(t+\phi))P(\alpha;\ t+\phi) \tag{10}$$

where $P(\alpha;t)$ is a T-periodic vector function. Here μ is to be the vector $(\mu_1,\mu_2,\ldots,\mu_{N-1})$; $\alpha\cdot\mu$ is the usual dot product. The proof is by induction on α , which is clearly possible even though the α's are not linearly ordered. Notice that (10) has already been verified for $|\alpha| = 0,1$.

For $|\alpha| \geq 2$, assuming (10) holds for $\beta<\alpha$, and using the homogeneity property of F_α , (3b), (8c) becomes:

$$U'(\alpha;t) = \nabla F(Q(t+\phi))U(\alpha;t) + \exp(-\alpha\cdot\mu(t+\phi))F_\alpha(P(\beta;\ t+\phi):\ \beta<\alpha). \tag{11}$$

Using the fundamental matrix of (6), the solutions of the general equation:

$$W' = \nabla F(Q(t))W + \exp(-\alpha\cdot\mu t)K(t)$$

can be written as (C = constant vector)

$$W = P(t)\exp(-Dt)\left[C + \int_0^t \exp(D-\alpha\cdot\mu I)s)P^{-1}(s)K(s)ds\right].$$

We are led to define (using Lemma A) a T-periodic vector $\hat{F}_\alpha(t)$:

$$-\hat{F}_\alpha(0)+\exp(D-\alpha\cdot\mu I)t)\hat{F}_\alpha(t) = \int_0^t \exp((D-\alpha\cdot\mu I)s)P^{-1}(s)F_\alpha(P_\beta(s):\beta<\alpha)ds. \tag{12}$$

and note that we must assume $\mathrm{Re}(\mu_i-\alpha\cdot\mu)\neq 0$, $i=1,2,\ldots,N-1$, hence, <u>the general assumption</u>: $\mathrm{Re}(j\mu_i)\neq\mathrm{Re}(\alpha\cdot\mu)$ for all integer vectors α, $|\alpha|\geq 2$.

Use of the general solution together with the definition of (12) shows that a solution of (11) can be found in the form

$$\begin{aligned} U(\alpha;t) &= \exp(-\alpha\cdot\mu(t+\phi))P(t+\phi)\hat{F}_\alpha(t+\phi) \\ &= \exp(-\alpha\cdot\mu(t+\phi))P(\alpha;t+\phi) \end{aligned} \tag{13}$$

with $P(t)\hat{F}_\alpha(t)$ T-periodic as claimed.

At this point, all necessary notation has been introduced, all formal calculations are completed, and all necessary assumptions have been mentioned. Before beginning the work on convergence, we state the full theorem to be proved in this section.

THEOREM 1.

Assume:

(1) $F(U)$ is analytic at each point of the limit cycle $U = Q(t)$, $0 \leq t \leq T$.

(2) In the Floquet representation $P(t)\exp(-Bt)$, $P(t)$ T- periodic, for a fundamental matrix of the variational equation (5), the constant matrix B is simple and has eigenvalues: $0, -\mu_1, \ldots, -\mu_{N-1})$, $\mathrm{Re}(\mu_i) > 0$.

(3) The $N-1$ nonzero eigenvalues μ_i satisfy

$$\mathrm{Re}\left(\mu_i - \sum_{j=1}^{N-1} \alpha_j \mu_j\right) \neq 0 \quad \text{for} \quad i = 1, \ldots, N-1$$

and all sets $\alpha_1, \alpha_2, \ldots, \alpha_{N-1}$ of non-negative integers with $\sum \alpha_i \geq 2$.

Then the solutions $U(t)$ of (4) can be written formally in terms of the expansion parameters $E = (e_1, e_2, \ldots, e_{N-1})$ as

$$U(t) = \sum_{n=0} \sum_{|\alpha|=n} \exp(-\alpha \cdot \mu t) P(\alpha; t+\phi) E^{\alpha}, \tag{14}$$

with $P(\alpha; t)$ T-periodic and given by (12), (13). The series converges for $|e_i|$, $i = 1, \ldots, N-1$ sufficiently small.

Hypothesis (1) on the analyticity of $F(U)$ has only been used so far in formal calculations; its real importance is in the proof of convergence. Hypothesis (2) is just a statement of the diagonalization assumption of (6); hypothesis (3) occurred in connection with (12). The formal calculation of (14) has been completed; all that is left to prove of Theorem 1 is the convergence of (14).

The matrix norm

$$||A|| = \max_i \sum_j |a_i^j| .$$

is used in the following discussion; for vector A, of course, it reduces to $\max_i |a_i|$.

The first step in proving convergence of (14) is to obtain a bound on the periodic coefficients $P(\alpha;t)$. Consider (12) and set:

$$G(t) = P^{-1}(t)F_\alpha(P(\beta;t): \beta < \alpha) = (g_1(t), \ldots, g_N(t)).$$

In (12) the i^{th} component has the form $(i = 1,\ldots,N; \mu_0 = 0)$

$$\int_0^t \exp((\mu_{i-1} - \alpha\cdot\mu)s)g_i(s)ds = \exp((\mu_{i-1} - \alpha\cdot\mu)t)\hat{F}_{\alpha,i}(t) - \hat{F}_{\alpha,i}(0) .$$

Using Lemma A.2 to estimate $\hat{F}_{\alpha,i}(t)$:

$$\sup_{[0,T]} |\hat{F}_{\alpha,i}(t)| \leq \left[\frac{1}{T}\int_0^T |g_i(s)|^2 ds\right]^{1/2}$$

$$\left[\frac{1}{|\mathrm{Re}(\mu_{i-1} - \alpha\cdot\mu)|^2 + |\frac{2\pi n}{T} - \mathrm{Im}(\mu_{i-1} - \alpha\cdot\mu)|^2}\right]^{1/2},$$

where the key point about the infinite sum on the right side is that the infinite sum $\rightarrow 0$ as $|\alpha| \rightarrow +\infty$. Consequently, the infinite sum can be bounded by a constant a_0, independent of α. Thus, noting $|g_i(t)| \leq |P^{-1}(t)F_\alpha|$,

$$\sup_{[0,T]} |\hat{F}_{\alpha,i}| \leq a_0 \sup_{[0,T]} |g_i(t)|$$

$$\leq a_0 \sup_{[0,T]} ||P^{-1}(t)|| \sup_{[0,T]} |F_\alpha(P(\beta;t):\beta<\alpha)| \quad .$$

Since $||P(\alpha;t)|| \leq ||P(t)|| \; ||\hat{F}_\alpha(t)||$ by (13), we finally have

$$\sup_{[0,T]} ||P(\alpha;t)|| \leq k \sup_{[0,T]} ||F_\alpha(P(\beta;t):\beta<\alpha)||, \tag{15}$$

where

$$k = a_0 \sup_{[0,T]} ||P(t)|| \sup_{[0,T]} ||P^{-1}(t)||,$$

independent of α,t.

The second step in proving convergence of (14) is the derivation of a majorant series for $F(U)$ in a neighborhood of the limit cycle.

For a scalar function $f(U)$, $U = (u_1,\ldots,u_N)$, analytic at a point $U = A$, a majorant series for $f(U)$ at A is a function $\hat{f}(U)$ analytic at A such that $|B(\alpha)| \leq C(\alpha)$, where $B(\alpha), C(\alpha)$ are the coefficients in their expansions about A:

$$f(U) = \sum_{n=0}^{\infty} \sum_{|\alpha| = n} B(\alpha)(U - A)^{\alpha}, \quad \hat{f}(U) = \sum_{n=0}^{\infty} \sum_{|\alpha| = n} C(\alpha)(U - A)^{\alpha} .$$

An important property of majorant series is connected with composition: let $f(U)$ have the majorant $\hat{f}(U)$ at $U = A$, and let two series be given, $E = (e_1,\ldots,e_M)$,

$$U = A + \sum_{n=1}^{\infty} \sum_{|\alpha| = n} U(\alpha)E^{\alpha} , \qquad V = A + \sum_{n=1}^{\infty} \sum_{|\alpha| = n} V(\alpha)E^{\alpha} ,$$

such that $|u_i(\alpha)| \leq v_i(\alpha)$ for the components of $U(\alpha), V(\alpha)$, $|\alpha| \geq 1$. Then, in the composites:

$$f(U) = f(A) + \sum_{|\alpha| = 1} \nabla f(A)U(\alpha)E^{\alpha} + \sum_{n=2}^{\infty} \sum_{|\alpha| = n} \left[\nabla f(A)U(\alpha) + f_{\alpha}(U(\beta): \beta < \alpha)\right] E^{\alpha},$$

$$\hat{f}(V) = \hat{f}(A) + \sum_{|\alpha| = 1} \nabla \hat{f}(A)V(\alpha)E^{\alpha} + \sum_{n=2}^{\infty} \sum_{|\alpha| = n} \left[\hat{f}(A)V(\alpha) + \hat{f}_{\alpha}(V(\beta): \beta < \alpha)\right] E^{\alpha}$$

we have

$$|f_\alpha(U(\rho):\ \rho < \alpha| \le \hat{f}_\alpha(V(\rho):\ \rho < \alpha), \qquad |\alpha| \ge 2. \tag{16}$$

The inequality holds because all coefficients in $f_\alpha(U(\rho):\ \rho < \alpha)$, which are only <u>sums</u> of monomials formed from coefficients in $f(U)$, have been replaced in $\hat{f}_\alpha(V(\rho);\ \rho < \alpha)$ by the corresponding sums of monomials formed from the nonnegative coefficients in $\hat{f}(U)$, and because the terms in $U(\rho)$ have been replaced by the nonnegative terms in $V(\rho)$.

A vector function $F(U)$ has $\hat{f}(U)$ for a majorant series at $U=A$ if $\hat{f}(U)$ is a majorant for each component $f_i(U)$ at $U=A$.

A majorant can always be chosen in a particularly simple form. If $f(U)$ is analytic at A, then

$$f(U) = \sum_{n=0}^{\infty} \sum_{|\alpha|=n} B(\alpha)(U-A)^\alpha = \sum_{n=0}^{\infty} \sum_{|\alpha|=n} \frac{1}{\alpha!} \frac{\partial^{|\alpha|} f}{\partial U^\alpha}(A)(U-A)^\alpha , \tag{17a}$$

where

$$\alpha! = \alpha_1!\,\alpha_2!\,\ldots\,\alpha_N! \qquad \text{and} \qquad \frac{\partial^{|\alpha|} f}{\partial U^\alpha} = \frac{\partial^{|\alpha|} f}{\partial u_1^{\alpha_1}\,\partial u_2^{\alpha_2}\,\ldots\,\partial u_N^{\alpha_N}} .$$

Let R_i be the radius of convergence of $f(U)$ with respect to u_i and choose $0 < R < R_i$, $i=1,\ldots,N$ (R, R_i scalars, of course).

Then, by Cauchy's Integral Theorem for several variables (Cartan, 1963, Chapter 4)

$$B(\alpha) = \frac{1}{\alpha!}\frac{\partial^{|\alpha|} f}{\partial U^{\alpha}}(A) = \frac{1}{(2\pi i)^{|\alpha|}} \int_{\substack{|z_i - a_i| = R \\ i=1,\ldots,N}} \frac{f(Z)\, dz_1 \ldots dz_N}{(z_1-a_1)^{\alpha_1+1} \ldots (z_N-a_N)^{\alpha_N+1}} ,$$

consequently,

$$|B(\alpha)| \leq \frac{1}{R^{|\alpha|}} \sup_{\substack{|z_i - a_i| = R \\ i=1,\ldots,N}} |f(Z)| \quad . \tag{17b}$$

It follows that at $U=A$, $f(U)$ has the majorant

$$\hat{f}(U) = c \prod_{i=1}^{N} \left(1 - \frac{u_i - a_i}{R}\right)^{-1} \quad .$$

In the convergence proof for Theorem 1, we used a majorant series, independent of t, for $F(U)$ at each point $U = Q(t)$ of the limit cycle. To find such a majorant, first note that at each point $Q(t)$, $0 \leq t \leq T$, there is an open ball within which $F(U)$ is analytic. Since $Q(T)$ is a smooth mapping, the curve $Q(t)$, $0 \leq t \leq T$, is compact and can be covered with finitely many such balls. Therefore, there exists an $R > 0$ such that $F(U)$, expanded as a series about a point $Q(t)$ converges in an open set containing $||U-Q(t)|| \leq R$ for arbitrary t, $0 \leq t \leq T$.

Expanding $F(U)$ around a point $U = Q(t)$, $0 \le t \le T$, gives

$$F(U) = \sum_{n=0}^{\infty} \sum_{|\alpha|=n} B(\alpha;\ t)(U - Q(t))^{\alpha} \quad , \tag{18a}$$

where, by (17b),

$$\| B(\alpha;\ t) \| \le \frac{1}{R^{|\alpha|}} \sup_{\substack{|z_i - Q_i(t)| = R \\ i=1,\dots,N}} \| F(Z) \| \quad .$$

Consequently,

$$\| B(\alpha;\ t) \| \le \frac{1}{R^{|\alpha|}} \sup_{\substack{|z_i - Q_i(t)| = R \\ i=1,\dots,N \\ 0 \le t \le T}} \| F(Z) \| \quad ,$$

and the upper bound on the right exists because the supremum is taken for a continuous function over a compact set. Therefore, <u>there exists a constant c, independent of t</u>, such that

$$\| B(\alpha;\ t) \| \le \frac{c}{R^{|\alpha|}} \quad , \tag{18b}$$

equivalently, $F(U)$ has a majorant series at each point $Q(t)$, $0 \le t \le T$, of the limit cycle and the majorant

$$\hat{f}(U) = c \prod_{i=1}^{N} \left(1 - \frac{u_i - q_i(t)}{R} \right)^{-1} \quad , \tag{18c}$$

has c, R independent of t.

These two basic points, the recursive bound (15) and the majorant (18), will be linked together by Lemma 2 below to give the convergence result. The proof of Lemma 2, however, will require a slight generalization of Liapunov's Lemma (which is Lemma 1 with $M=1$, see Lefschetz, 1977, Chapter 5):

LEMMA 1. Let $\hat{\hat{f}}(u) = c(1-u/R)^{-N}$, and let $u = \sum_{n=1}^{\infty} \sum_{|\alpha|=n} b(\alpha)E^{\alpha}$, $E = (e_1, \ldots, e_M)$, so that

$$\hat{\hat{f}}(u) = \hat{\hat{f}}(0) + \sum_{|\alpha|=1} \hat{\hat{f}}'(0)b(\alpha)E^{\alpha}$$
$$+ \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \left[\hat{\hat{f}}'(0)b(\alpha) + \hat{\hat{f}}_{\alpha}(b(\beta)\colon \beta < \alpha)\right]E^{\alpha} \,. \tag{19}$$

If $|b(\alpha)| \le k\,|\hat{\hat{f}}\,(b(\beta)\colon \beta < \alpha)|$, then $\sum_{n=1}^{\infty} \sum_{|\alpha|=n} b(\alpha)E^{\alpha}$ converges for $||E|| < d$, where d depends only on c, k, R, N.

PROOF: From the series expansion (19), notice that

$$\hat{\hat{f}}(u) - \hat{\hat{f}}(0) - \hat{\hat{f}}'(0)u = \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \hat{\hat{f}}_{\alpha}(b(\beta)\colon \beta < \alpha)E^{\alpha}.$$

Next, noticing $\sum_{|\alpha|=1} b(\alpha)E^{\alpha} = \sum_{i=1} b_i e_i$, where $b_1 = b(1,0,\ldots,0)$, $b_2 = b(0,1,0,\ldots,0)$, etc., consider

$$g(u,e_1,\ldots,e_M) = \sum_{i=1}^{N} |b_i|\, e_i - u + \bar{k}\left[\hat{\hat{f}}(u) - \hat{\hat{f}}(0) - \hat{\hat{f}}'(0)u\right] = 0.$$

Clearly g is an analytic function of $u, e_1, \ldots, e_M$ and at $u, e_1, \ldots, e_M = 0, 0, \ldots, 0$, $\frac{\partial g}{\partial u} \neq 0$. By the implicit function theorem for complex variables (Lefschetz, 1977, Chapter 1; a proof in the simplest case $f(z,w) = 0$ is in Evgrafov, 1978, Chapter 4), $u = u(e_1, \ldots, e_M)$ exists as an analytic solution of $g(u, e_1, \ldots, e_M) = 0$ in a neighborhood of the point $(0, 0, \ldots, 0)$. Substitution of

$$u = \sum_{n=1}^{\infty} \sum_{|\alpha|=n} c(\alpha) E^{\alpha}$$

into $g = 0$ gives

$$c(\alpha) = |b(\alpha)|, \quad |\alpha| = 1,$$

and

$$c(\alpha) = k\hat{\hat{f}}_{\alpha}(c(\beta) : \beta < \alpha),$$

from which $c(\alpha) \geq |b(\alpha)|$ for all α follows, giving a majorant for the $b(\alpha)$-series. Q.E.D.

LEMMA 2.

Assume:

(1) $F(U)$ is analytic at each point $U = Q(t)$, $0 \leq t \leq T$, with a majorant independent of t,

$$\hat{f}(U) = c \prod \left(1 - \frac{u_i - q_i(t)}{R}\right)^{-1} .$$

(2) $\sum_{n=1}^{\infty} \sum_{|\alpha|=n} P(\alpha;t)E^{\alpha}$ with $0 \leq t \leq T$ and $E = (e_1,\ldots,e_M)$

is a series whose coefficients satisfy

$$||P(\alpha;t)|| \leq k \sup_{[0,T]} ||F_{\alpha}(P(\beta;t): \beta < \alpha)||,$$

where the F_{α} arise by setting

$$U = Q(t) + \sum_{n=1}^{\infty} \sum_{|\alpha|=n} P(\alpha;t)E^{\alpha}$$

to give

$$F(U) = F(Q(t)) + \sum_{|\alpha|=1} \nabla F(Q(t))P(\alpha;t)E^{\alpha}$$
$$+ \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \left[\nabla F(Q(t))P(\alpha;t)+F_{\alpha}(P(\beta;t): \beta<\alpha)\right] E^{\alpha}.$$

Then, $\sum_{n=1}^{\infty} \sum_{|\alpha|=n} P(\alpha;t)E^{\alpha}$ converges absolutely and uniformly on $0 \leq t \leq T$ for $||E|| < d$, where d depends only on c,R,k,N.

PROOF:

First, for $|\alpha| \geq 1$, let $B(\alpha)$ be n-vectors with identical components,

$$b_i(\alpha) = b(\alpha) = \sup_{[0,T]} ||P(\alpha,t)||.$$

Substitution into the majorant $\hat{f}(U)$ of

$$B = Q(t) + \sum_{n=1}^{\infty} \sum_{|\alpha|=n} B(\alpha)E^{\alpha}$$

gives

$$\begin{aligned} \hat{f}(B) &= \hat{f}(Q(t)) + \sum_{|\alpha|=1} \nabla\hat{f}(Q(t))B(\alpha)E^{\alpha} \\ &\quad + \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \left[\nabla\hat{f}(Q(t))B(\alpha) + \hat{f}_{\alpha}(B(\beta)\colon\ \beta < \alpha)\right]E^{\alpha} . \end{aligned} \tag{20a}$$

The property (16) allows us to compare F_{α} and $\hat{f}_{\alpha}$:

$$\| F_{\alpha}(P(\beta;t)\colon\ \beta < \alpha) \| \leq \hat{f}_{\alpha}(B(\beta)\colon\ \beta < \alpha) ,$$

and using hypothesis (2) of the Lemma gives

$$\| F(\alpha;t) \| \leq k\hat{f}_{\alpha}(B(\beta)\colon\ \beta < \alpha). \tag{20b}$$

Notice that

$$\begin{aligned} &\hat{f}(B) - \hat{f}(Q(t)) - \sum_{n=1}^{\infty} \sum_{|\alpha|=n} \nabla\hat{f}(Q(t))B(\alpha)E^{\alpha} \\ &\quad = c\left(\left(1 - \frac{b}{R}\right)^{-N} - 1 - \frac{N}{R}\,b\right) , \end{aligned} \tag{20c}$$

where

$$b = \sum_{n=1}^{\infty} \sum_{|\alpha|=n} b(\alpha)E^{\alpha} .$$

If $\hat{f}(u) = c(1-u/R)^{-N}$, then

$$\hat{\hat{f}}(b) = \hat{\hat{f}}(0) + \sum_{|\alpha|=1} \hat{\hat{f}}'(0)b(\alpha)E^{\alpha}$$

$$+ \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \left[\hat{\hat{f}}'(0)b(\alpha) + \hat{\hat{f}}_{\alpha}(b(\beta):\ \beta < \alpha)\right] E^{\alpha} ,$$

so,

$$c\ (1 - \frac{b}{R})^{-N} - 1 - N\frac{b}{R} = \sum_{n=2}^{\infty} \sum_{|\alpha|=n} \left[\hat{\hat{f}}_{\alpha}(b(\beta):\ \beta < \alpha)\right] E^{\alpha} . \tag{20d}$$

Combining (20a), (20c), and (20d), gives

$$\hat{f}_{\alpha}(B(\beta):\ \beta < \alpha) = \hat{\hat{f}}_{\alpha}(b(\beta):\ \beta < \alpha)$$

and inserting this equality into (20b) gives

$$b(\alpha) \leq k\hat{\hat{f}}_{\alpha}(b(\beta):\ \beta < \alpha).$$

Applying Lemma 1 to the last inequality gives convergence of $\sum b(\alpha)E^{\alpha}$ for $||E|| < d$, where d depends only on $c,k,R,N,$ which is a t-independent majorant for $\sum P(\alpha;t)E^{\alpha}$. Q.E.D.

Finally, the majorant of (18) satisfies the first hypothesis and the bounds (15) satisfy the second hypothesis of Lemma 2, and the absolute convergence of $\sum P(\alpha;t)E^{\alpha}$ forces convergence of (14). This proves Theorem 1.

APPENDIX III

HIGHER-ORDER TERMS OF THE EXPANSION IN CHAPTER IV

This appendix derives the higher-order terms $u_n, v_n, n \geq 3$, and gives an inductive proof of the properties listed in (IV.2.2c).

The terms u_n, v_n are basically determined by the coefficient of ϵ^n in the expansion (IV.2.1d); this coefficient is

$$\begin{bmatrix} u_{n\theta} \\ v_{n\theta} \end{bmatrix} = \begin{bmatrix} F_u(U,V) & F_v(U,V) \\ G_u(U,V) & G_v(U,V) \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} + \left[\begin{matrix} -u_{n-1,\tau} + (1+\alpha)\nabla^2 u_{n-1} \\ -v_{n-1,\tau} + (1-\alpha)\nabla^2 v_{n-1} \end{matrix}\right.$$

$$+ \sum_{k+\ell=n-1} (-u_{k\theta}\phi_{\ell\tau} + (1+\alpha)(u_{k\theta}\nabla^2\phi_\ell + 2\nabla u_{k\theta}\cdot\nabla\phi_\ell))$$

$$+ \sum_{k+\ell=n-1} (-v_{k\theta}\phi_{\ell\tau} + (1-\alpha)(v_{k\theta}\nabla^2\phi_\ell + 2\nabla v_{k\theta}\cdot\nabla\phi_\ell))$$

$$\left.\begin{matrix} +(1+\alpha) \sum_{k+\ell+m=n-1} (u_{k\theta\theta}\nabla\phi_\ell\cdot\nabla\phi_m) \\ +(1-\alpha) \sum_{k+\ell+m=n-1} (v_{k\theta\theta}\nabla\phi_\ell\cdot\nabla\phi_m) \end{matrix}\right] \qquad \text{(term \#1)}$$

$$+ \begin{bmatrix} F_n(u_0,\ldots,u_{n-1},v_0,\ldots,v_{n-1}) \\ G_n(u_0,\ldots,u_{n-1},v_0,\ldots,v_{n-1}) \end{bmatrix} \qquad \text{(term \#2).}$$

The first order of business is to separate out all terms containing the functions ϕ_{n-1}, B_{n-1}. By induction and (IV.2.2c.6) the terms $u_0, v_0, \ldots, u_{n-1}, v_{n-1}$ do not depend on ϕ_{n-1}; B_{n-1} only occurs in u_{n-1}, v_{n-1}. We split Term #1 in (1) into the following parts:

$$(\#1) = (\#1a) + (\#1b) + (\#1c) , \tag{2a}$$

$$(\#1a) = \begin{bmatrix} (-\phi_{n-1,\tau} + (1+\alpha)\nabla^2\phi_{n-1})U'(\theta) + 2(1+\alpha)\nabla\phi_0 \cdot \nabla\phi_{n-1} U''(\theta) \\ (-\phi_{n-1,\tau} + (1-\alpha)\nabla^2\phi_{n-1})V'(\theta) + 2(1-\alpha)\nabla\phi_0 \cdot \nabla\phi_{n-1} V''(\theta) \end{bmatrix}$$

$$(\#1b) = \begin{bmatrix} -u_{n-1,\tau} + (1+\alpha)\nabla^2 u_{n-1} - \phi_{0\tau} u_{n-1,\theta} + (1+\alpha) \\ -v_{n-1,\tau} + (1-\alpha)\nabla^2 v_{n-1} - \phi_{0\tau} v_{n-1,\theta} + (1-\alpha) \end{bmatrix.$$

$$\begin{matrix} (u_{n-1,\theta}\nabla^2\phi_0 + 2\nabla u_{n-1,\theta} \cdot \nabla\phi_0 + |\nabla\phi_0|^2 u_{n-1,\theta\theta}) \\ (v_{n-1,\theta}\nabla^2\phi_0 + 2\nabla v_{n-1,\theta} \cdot \nabla\phi_0 + |\nabla\phi_0|^2 v_{n-1,\theta\theta}) \end{matrix}\Bigg]$$

$$(\#1c) = \left[\begin{array}{l} + \sum\limits_{\substack{k+\ell=n-1 \\ k,\ell\neq 0}} (-u_{k\theta}\phi_{\ell\tau} + (1+\alpha)(u_{k\theta}\nabla^2\phi_\ell + 2\nabla u_{k\theta}\cdot\nabla\phi_\ell)) \\ + \sum\limits_{\substack{k+\ell=n-1 \\ k,\ell\neq 0}} (-v_{k\theta}\phi_{\ell\tau} + (1-\alpha)(v_{k\theta}\nabla^2\phi_\ell + 2\nabla v_{k\theta}\cdot\nabla\phi_\ell)) \\ \qquad + (1+\alpha) \sum\limits_{\substack{k+\ell+m=n-1 \\ k,\ell,m\neq 0}} u_{k\theta\theta}\nabla\phi_\ell\cdot\nabla\phi_m \\ \qquad + (1-\alpha) \sum\limits_{\substack{k+\ell+m=n-1 \\ k,\ell,m\neq 0}} v_{k\theta\theta}\nabla\phi_\ell\cdot\nabla\phi_m \end{array} \right]$$

Here ϕ_{n-1} occurs in (#1a) only; B_{n-1} occurs in (#1b) only; *(#1c) consists solely of known terms.*

To find the explicit dependence of (#1b) on B_{n-1}, we substitute u_{n-1}, v_{n-1} as given by (IV.2.2c.5) into (#1c), obtaining:

$$
(\#1b) = \exp(-\mu\theta)
\begin{bmatrix}
\Big(-B_{n-1,\tau}+(1+\alpha)\nabla^2 B_{n-1}-2\mu(1+\alpha)\nabla\phi_0\cdot\nabla B_{n-1} \\
\quad +\mu\phi_{0\tau}+(1+\alpha)(-\mu\nabla^2\phi_0+\mu^2|\nabla\phi_0|^2))B_{n-1}\Big)\hat{U}(\theta) \\
+(2(1+\alpha)\nabla\phi_0\cdot\nabla B_{n-1}+(-\phi_{0\tau}+(1+\alpha)(\nabla^2\phi_0-2\mu|\nabla\phi_0|^2))B_{n-1})\hat{U}'(\theta) \\
\quad +(1+\alpha)|\nabla\phi_0|^2 B_{n-1}\hat{U}''(\theta) \\
\\
\Big(-B_{n-1,\tau}+(1-\alpha)\nabla^2 B_{n-1}-2\mu(1-\alpha)\nabla\phi_0\cdot\nabla B_{n-1} \\
\quad +\mu\phi_{0\tau}+(1+\alpha)(-\mu\nabla^2\phi_0+\mu^2|\nabla\phi_0|^2))B_{n-1}\Big)\hat{V}(\theta) \\
+(2(1-\alpha)\nabla\phi_0\cdot\nabla B_{n-1}+(-\phi_{0\tau}+(1-\alpha)(\nabla^2\phi_0-2\mu|\nabla\phi_0|^2))B_{n-1})\hat{V}'(\theta) \\
\quad +(1-\alpha)|\nabla\phi_0|^2 B_{n-1}\hat{V}''(\theta)
\end{bmatrix} \qquad (2b)
$$

$+$ [Known remainder terms in u_{n-1},v_{n-1}]

Term #2 in (1) will now be considered. As noted above, ϕ_{n-1} will not occur in F_n,G_n; however, B_{n-1} will occur in the terms containing u_{n-1},v_{n-1}. The following lemma gives the dependence of F_n,G_n on u_{n-1},v_{n-1}:

LEMMA 1. Given $F(u,v)$, $u = \sum_{n=0}^{\infty} u_n \epsilon^n$, $v = \sum_{n=0}^{\infty} v_n \epsilon^n$ so that:

$$F(u,v) = F(u_0,v_0) + [F_u(u_0,v_0)u_1 + F_v(u_0,v_0)v_1]\epsilon$$
$$+ \sum_{n=2}^{\infty} [F_u(u_0,v_0)u_n + F_v(u_0,v_0)v_n$$
$$+ F_n(u_0,u_1,\ldots,u_{n-1},\ v_0,v_1,\ldots,v_{n-1})]\,\epsilon^n$$

then:

(a)
$$F_2(u_0,u_1,v_0,v_1) = \frac{1}{2}\left[F_{uu}(u_0,v_0)u_1^2+2F_{uv}(u_0v_0)u_1v_1+F_{vv}(u_0,v_0)v_1^2\right],$$

(b)
$$F_n(u_0,\ldots,u_{n-1},\ v_0,\ldots,v_{n-1})$$

$$= F_{uu}(u_0,v_0)u_1u_{n-1}+F_{uv}(u_0,v_0)(u_1v_{n-1}+v_1u_{n-1})+F_{vv}(u_0,v_0)v_1v_{n-1}$$

$$+ F_n(u_0,\ldots,u_{n-2},\ v_0,\ldots,v_{n-2}),\quad n \geq 3.$$

PROOF: For $n \geq 2$, notice

$$F_u(u_0,v_0)u_n+F_v(u_0,v_0)v_n+F_n = \frac{1}{n!}\left(\frac{d}{d\epsilon}\right)^n (F(u,v))\Bigg|_{\epsilon=0}$$

$$= \frac{1}{n!}\left(\frac{d}{d\epsilon}\right)^{n-2}(F_uu_{\epsilon\epsilon}+F_vv_{\epsilon\epsilon}+F_{uu}u_\epsilon^2+2F_{uv}u_\epsilon v_\epsilon+F_{vv}v_\epsilon^2)\Bigg|_{\epsilon=0}$$

If $n=2$, then (a) follows immediately. If $n \geq 3$, then Leibniz' rule for differentiating products gives:

$$= \frac{1}{n!}\Big[F_u u_{\epsilon^n} + F_v v_{\epsilon^n} + (n-2)\Big[(F_{uu}u_\epsilon + F_{uv}v_\epsilon)u_{\epsilon^{n-1}} + (F_{uv}u_\epsilon + F_{vv}v_\epsilon)v_{\epsilon^{n-1}}\Big]$$
$$+ \dots + 2\Big[F_{uu}u_\epsilon u_{\epsilon^{n-1}} + F_{uv}(u_\epsilon v_{\epsilon^{n-1}} + v_\epsilon u_{\epsilon^{n-1}}) + F_{vv}v_\epsilon v_{\epsilon^{n-1}}\Big] + \dots\Big]_{\epsilon=0}$$

where only terms containing ϵ-derivatives of order $n-1$ or n have been kept. Setting $\epsilon=0$ gives (b). Q.E.D.

Using Lemma 1 to obtain the explicit occurrence of B_{n-1} in Term #2 gives:

$$\text{Term\#2} = \begin{bmatrix} (F_{uu}(U,V)u_1 + F_{uv}(U,V)v_1)\hat{U} + (F_{uv}(U,V)u_1 + F_{vv}(U,V)v_1)\hat{V} \\ \\ (G_{uu}(U,V)u_1 + G_{uv}(U,V)v_1)\hat{U} + (G_{uv}(U,V)u_1 + G_{vv}(U,V)v_1)\hat{V} \end{bmatrix} B_{n-1}\exp(-\mu\theta)$$

$$+ \text{ known remainder terms in } u_0, v_0, \dots, u_{n-1}, v_{n-1} \quad .$$

In order to prove statements like (IV.2.2c.6) on the structure of the terms in u_n, v_n, it is necessary to know something about the structure of the remainer terms in (#1b), (#1c), and (#2). Using induction and (IV.2.2c.5,6), we know the structure of the terms $u_0, v_0, \dots, u_{n-1}, v_{n-1}$; and from this information we can make the following observations about the known remainder terms in each of (#1b), (#1c), and (#2), and consequently for their sum which will be represented by (3a):

(3a) The remainder term is a polynomial in the exponential terms $\exp(-\mu\theta)$ of order $n-1$, and can be written as:

$$\sum_{k=0}^{n-1} \begin{bmatrix} R_k(\tau,\underset{\sim}{\xi},\theta) \\ S_k(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} \exp(-k\mu\theta) ,$$

where each coefficient R_k, S_k is T-periodic in θ.

(3b) Each R_k, S_k is a linear combination of T-periodic terms in θ with coefficients depending on the $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau,\underset{\sim}{\xi}),\ldots,\phi_{n-2}(\tau,\underset{\sim}{\xi})$, functions of $\phi_0(0,\underset{\sim}{\xi})$, and the functions $B_1,\ldots,B_{n-2}$ and their derivatives.

(3c) In particular, the $R_0(\tau,\underset{\sim}{\xi},\theta)$, $S_0(\tau,\underset{\sim}{\xi},\theta)$ term is independent of the $B_1,\ldots,B_{n-2}$ terms and the coefficients of the T-periodic terms are polynomials in the $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau,\underset{\sim}{\xi}),\ldots,\phi_{n-2}(\tau,\underset{\sim}{\xi})$ and functions of $\phi_0(0,\underset{\sim}{\xi})$; and these coefficients are such that if the $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau,\underset{\sim}{\xi}),\ldots,\phi_{n-2}(\tau,\underset{\sim}{\xi})\to 0$ as $\tau\to+\infty$, then $R_0,S_0\to 0$ also.

(In regard to (3c), no B_k can appear in R_0,S_0 simply because each B_k when it first appears is part of the product $B_k\exp(-\mu\theta)$, and in all operations - differentiation, multiplication, the integration below - nothing is ever done to separate such a product.)

Using (3a) to represent the general sum of the known remainder terms in (#1b), (#1c), and (#2), the equation (1) can now be written, showing the complete dependence on ϕ_{n-1}, B_{n-1} as:

$$\begin{bmatrix} u_{n\theta} \\ v_{n\theta} \end{bmatrix} = \begin{bmatrix} F_u(U,V) & F_v(U,V) \\ G_u(U,V) & G_v(U,V) \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} \tag{4}$$

$$+ \begin{bmatrix} (-\phi_{n-1,\tau}+(1+\alpha)\nabla^2\phi_{n-1})U'(\theta)+2(1+\alpha)\nabla\phi_0\cdot\nabla\phi_{n-1}U''(\theta) \\ (-\phi_{n-1,\tau}+(1-\alpha)\nabla^2\phi_{n-1})V'(\theta)+2(1-\alpha)\nabla\phi_0\cdot\nabla\phi_{n-1}V''(\theta) \end{bmatrix}$$

$$+ \exp(-\mu\theta) \begin{bmatrix} \begin{aligned} &\Big(-B_{n-1,\tau}+(1+\alpha)\nabla^2 B_{n-1}-2\mu(1+\alpha)\nabla\phi_0\cdot\nabla B_{n-1} \\ &\qquad +\mu\phi_{0\tau}+(1+\alpha)(-\mu\nabla^2\phi_0+\mu^2|\nabla\phi_0|^2))B_{n-1}\Big)\hat{U}(\theta) \\ &+(2(1+\alpha)\nabla\phi_0\cdot\nabla B_{n-1}+(-\phi_{0\tau}+(1+\alpha)(\nabla^2\phi_0-2\mu|\nabla\phi_0|^2))B_{n-1})\hat{U}'(\theta) \\ &\qquad +(1+\alpha)|\nabla\phi_0|^2 B_{n-1}\hat{U}''(\theta) \\ \\ &\Big(-B_{n-1,\tau}+(1-\alpha)\nabla^2 B_{n-1}-2\mu(1-\alpha)\nabla\phi_0\cdot\nabla B_{n-1} \\ &\qquad +\mu\phi_{0\tau}+(1+\alpha)(-\mu\nabla^2\phi_0+\mu^2|\nabla\phi_0|^2))B_{n-1}\Big)\hat{V}(\theta) \\ &+(2(1-\alpha)\nabla\phi_0\cdot\nabla B_{n-1}+(-\phi_{0\tau}+(1-\alpha)(\nabla^2\phi_0-2\mu|\nabla\phi_0|^2))B_{n-1})\hat{V}'(\theta) \\ &\qquad +(1-\alpha)|\nabla\phi_0|^2 B_{n-1}\hat{V}''(\theta) \end{aligned} \end{bmatrix}$$

$$+ \begin{bmatrix} (F_{uu}(U,V)P_{10}(\tau,\underset{\sim}{\xi},\theta)+F_{uv}(U,V)Q_{10}(\tau,\underset{\sim}{\xi},\theta))\hat{U}(\theta) \\ (G_{uu}(U,V)P_{10}(\tau,\underset{\sim}{\xi},\theta)+G_{uv}(U,V)Q_{10}(\tau,\underset{\sim}{\xi},\theta))\hat{U}(\theta) \end{bmatrix}$$

$$+ \begin{bmatrix} + (F_{uv}(U,V)P_{10}(\tau,\underset{\sim}{\xi},\theta)+F_{vv}(U,V)Q_{10}(\tau,\underset{\sim}{\xi},\theta))\hat{V}(\theta) \\ + (G_{uv}(U,V)P_{10}(\tau,\underset{\sim}{\xi},\theta)+G_{vv}(U,V)Q_{10}(\tau,\underset{\sim}{\xi},\theta))\hat{V}(\theta) \end{bmatrix} B_{n-1}\exp(-\mu\theta)$$

$$+ \begin{bmatrix} F_{uu}(U,V)\hat{U}^2+2F_{uv}(U,V)\hat{U}\hat{V}+ F_{vv}(U,V)(\hat{V})^2 \\ G_{uu}(U,V)\hat{U}^2+2G_{uv}(U,V)\hat{U}\hat{V}+ G_{vv}(U,V)(\hat{V})^2 \end{bmatrix} \quad (B_1+f)B_{n-1}\exp(-2\mu\theta)$$

$$+ \sum_{k=0}^{n-1} \begin{bmatrix} R_k(\tau,\underset{\sim}{\xi},\theta) \\ S_k(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} \exp(-k\mu\theta) .$$

Notice the resemblance of the ϕ_{n-1} and B_{n-1} terms to those for ϕ_1 and B_1 (or $\hat{B} = B_1+f$) in (IV.2.7) and (IV.2.8). Applying Lemma D to (4), using the previous definitions (IV.2.5) and (IV.2.9), and defining

$$\frac{1}{T}\int_0^T \frac{R_0(\tau,\underset{\sim}{\xi},s)\hat{V}(s) - S_0(\tau,\underset{\sim}{\xi},s)\hat{U}(s)}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)}\, ds = h_{n-1}(\tau,\underset{\sim}{\xi}) \quad , \qquad (5)$$

$$\frac{1}{T}\int_0^T \left\{ \begin{aligned} &((G_{uu}(U,V)\hat{U} +G_{uv}(U,V)\hat{V})P_{10}(\tau,\underset{\sim}{\xi},s)+(G_{uv}(U,V)\hat{U} \\ &+ G_{vv}(U,V)\hat{V})Q_{10}(\tau,\underset{\sim}{\xi},s))\ U'(s) \\ &-((F_{uu}\hat{U}+F_{uv}\hat{V})P_{10}(\tau,\underset{\sim}{\xi},s)+(F_{uv}\hat{U}+F_{vv}\hat{V})Q_{10}(\tau,\underset{\sim}{\xi},s))\ V'(s) \end{aligned} \right\} \frac{ds}{U'\hat{V}-V'\hat{U}}$$

$$= f_{n-1}(\tau,\underset{\sim}{\xi}) \ ,$$

$$\frac{1}{T}\int_0^T \frac{S_1(\tau,\underset{\sim}{\xi},s)U'(s)-V'(s)R_1(\tau,\underset{\sim}{\xi},s)}{U'(s)\hat{V}(s) - V'(s)\hat{U}(s)}\,ds = \hat{h}_{n-1}(\tau,\underset{\sim}{\xi}) ,$$

we finally have:

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} = A_n(\tau,\underset{\sim}{\xi}) \begin{bmatrix} U'(\theta) \\ V'(\theta) \end{bmatrix} + B_n(\tau,\underset{\sim}{\xi})\exp(-\mu\theta) \begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix}$$

$$+ \left[\begin{matrix} (-\phi_{n-1,\tau}+(1+\alpha h_1)\nabla^2\phi_{n-1}+2(\ell_1+\alpha m_1)\nabla\phi_0\cdot\nabla\phi_{n-1}+h_{n-1}(\tau,\underset{\sim}{\xi}))\,\theta \\ \\ \begin{pmatrix} (-B_{n-1,\tau}+(1-\alpha h_1)\nabla^2 B_{n-1}+2(\ell_{21}+\alpha\ell_{22}-\mu(1-\alpha h_1))\nabla\phi_0\cdot\nabla B_{n-1} \\ +f_{n-1}(\tau,\underset{\sim}{\xi})B_{n-1}+\hat{h}_{n-1}(\tau,\underset{\sim}{\xi}) \end{pmatrix} \theta\exp(-\mu\theta) \end{matrix} \right]$$

$$+ \sum_{k=0}^{n} \begin{bmatrix} P_{nk}(\tau,\underset{\sim}{\xi},\theta) \\ Q_{nk}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} \exp(-k\mu\theta).$$

Setting the coefficients of θ, $\theta\exp(-\mu\theta)$ to 0 gives (IV.2.2c.1,3). The structural properties listed in (3) for the coefficients in R_0, S_0, R_1, S_1 together with the definitions in (5) give (IV.2.2c.2,4). Setting $A_n(\tau,\underset{\sim}{\xi}) = 0$ gives (IV.2.2c.5,7), and (IV.2.2c.6) follows from the structural properties listed in (3), which are not changed under the θ-integration resulting from applying Lemma D. This proves (IV.2.2c) for $n \geq 3$.

APPENDIX IV

AN ALTERNATE APPROACH TO THE EXPANSION OF CHAPTER IV FINITE SERIES FOR θ

In the derivation of the expansion in Section 2 of Chapter IV, it should be noticed that the original expression for u_1, v_1 (IV.2.6a) had the form

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = A_1(\tau,\underset{\sim}{\xi}) \begin{bmatrix} U'(\theta) \\ V'(\theta) \end{bmatrix} + \ldots \qquad .$$

The function $A_1(\tau,\underset{\sim}{\xi})$ was arbitrarily taken to be 0; the equation (IV.2.2c.1) for ϕ_1 resulting from the solution for u_2, v_2 was a consequence of this choice for A_1. It seems plausible that we might just as well have set $\phi_1 = 0$ and found an equation for A_1 -- this approach is investigated in this section.

In fact, instead of taking the sequence $A_n(\tau,\underset{\sim}{\xi})$ to be 0 (in equations (IV.2.10) and (6)) and then obtaining equations for ϕ_n, we could take each ϕ_n to be 0 and obtain an equation for A_n. In this way, only the finite series $t+\phi_0(\tau,\underset{\sim}{\xi})$ would be required for θ. However, in return for a simpler θ, the higher-order terms are more complicated. The study of these higher-order terms has not been pursued; this section will only derive an equation for A_1 to illustrate the idea. Since the equation for A_1 is not solvable and the equation for ϕ_1 is solvable, the expansion of Section 2 is preferable.

Briefly, the expansion of this section through $O(\epsilon)$ is:

$$\theta = t + \phi_0(\tau,\underset{\sim}{\xi}) + O(\epsilon^2) \ , \tag{1a}$$

where ϕ_0 *still satisfies* (IV.2.2b.1);

$$\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \begin{bmatrix} U(\theta) \\ V(\theta) \end{bmatrix} \tag{1b}$$

as in (IV.2.2a);

$$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = A_1(\tau,\underset{\sim}{\xi})\begin{bmatrix} U'(\theta) \\ V'(\theta) \end{bmatrix} + (B_1(\tau,\underset{\sim}{\xi}) + f(\tau,\underset{\sim}{\xi})\exp(-\mu\theta)\begin{bmatrix} \hat{U}(\theta) \\ \hat{V}(\theta) \end{bmatrix} + \begin{bmatrix} P_{10}(\tau,\underset{\sim}{\xi},\theta) \\ Q_{10}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} , \tag{1c}$$

where P_{10}, Q_{10}, f are the same functions as in (IV.2.2b), and A_1, B_1 are to be determined by u_2, v_2;

$$A_{1\tau} = (1+\alpha h_1)\nabla^2 A_1 + 2(\ell_1+\alpha m_1)\nabla\phi_0\cdot\nabla A_1 + g(\tau,\underset{\sim}{\xi})A_1 + \hat{h}(\tau,\underset{\sim}{\xi}) \ , \tag{1d}$$

where $g, \hat{h}$ are polynomials in $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau,\underset{\sim}{\xi})$ such that $g,\hat{h} \to 0$ if the $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau,\underset{\sim}{\xi})$ go to 0 as $\tau \to +\infty$.

If $\phi_0(\tau,\underset{\sim}{\xi})$ satisfies periodic initial data, then its $\underset{\sim}{\xi}$-derivatives decay exponentially fast in τ to 0, as shown by Lemma 1 of Section 3 in Chapter IV, so in (1d) $g(\tau,\underset{\sim}{\xi})$ and $\hat{h}(\tau,\underset{\sim}{\xi})$ decay exponentially fast in τ to 0. The arguments given for (IV.3.5) could now be repeated to show that

$$\int_0^P |A_1|^2 \, d\xi$$

remains bounded as $\tau \to +\infty$. In short, the only important difference between this approach and that of Section 2 appears to be the difference in solvability of (1d) and (IV.2.2c.1).

To obtain equation (1), all calculations of Section 2 through equation (IV.2.6a) can be carried out without change. Then (IV.2.2a) becomes (1b); (IV.2.6a) becomes (1c) when the θ-term is eliminated; eliminating the θ-term shows ϕ_0 satisfies (IV.2.2b.1), as mentioned in (1a). It only remains to derive (1d) by considering u_2, v_2.

The coefficient of ϵ^2 in (IV.2.1d) gives an equation for u_2, v_2; if $\phi_1 = 0$ this coefficient becomes (note (IV.2.7)):

$$\begin{bmatrix} u_{2\theta} \\ v_{2\theta} \end{bmatrix} = \begin{bmatrix} F_u(U,V) & F_v(U,V) \\ G_u(U,V) & G_v(U,V) \end{bmatrix} \begin{bmatrix} u_2 \\ v_2 \end{bmatrix} \tag{2a}$$

$$+ \begin{bmatrix} -u_{1\tau} - \phi_{0\tau} u_{1\theta} + (1+\alpha)(\nabla^2 u_1 + \nabla^2 \phi_0 u_{1\theta} + 2\nabla\phi_0 \cdot \nabla u_{1\theta} + |\nabla\phi_0|^2 u_{1\theta\theta}) \\ -v_{1\tau} - \phi_{0\tau} v_{1\theta} - (1-\alpha)(\nabla^2 v_1 + \nabla^2 \phi_0 v_{1\theta} + 2\nabla\phi_0 \cdot \nabla v_{1\theta} + |\nabla\phi_0|^2 v_{1\theta\theta}) \end{bmatrix}$$

$$+ \frac{1}{2} \begin{bmatrix} F_{uu}(U,V) u_1^2 + 2F_{uv}(U,V) u_1 v_1 + F_{vv}(U,V) v_1^2 \\ G_{uu}(U,V) u_1^2 + 2G_{uv}(U,V) u_1 v_1 + G_{vv}(U,V) v_1^2 \end{bmatrix} .$$

Now substitute u_1, v_1 as given by (1c). The nonhomogeneous terms will now contain functions periodic in θ and products of $\exp(-\mu\theta)$ and $\exp(-2\mu\theta)$ with periodic functions of θ. Rewriting (2) to show terms relevant to determining A_1 gives:

$$\begin{bmatrix} u_{2\theta} \\ v_{2\theta} \end{bmatrix} = \begin{bmatrix} F_u(U,V) & F_v(U,V) \\ G_u(U,V) & G_v(U,V) \end{bmatrix} \begin{bmatrix} u_2 \\ v_2 \end{bmatrix} \tag{2b}$$

$$+ \begin{bmatrix} -A_{1\tau}U' - \phi_{0\tau}A_1U'' + (1+\alpha)(\nabla^2 A_1 U' + (\nabla^2\phi_0 A_1 + 2\nabla\phi_0\cdot\nabla A_1)U'' + |\nabla\phi_0|^2 U''') \\ -A_{1\tau}V' - \phi_{0\tau}A_1V'' + (1-\alpha)(\nabla^2 A_1 V' + (\nabla^2\phi_0 A_1 + 2\nabla\phi_0\cdot\nabla A_1)V'' + |\nabla\phi_0|^2 V''') \end{bmatrix}$$

$$+ \begin{bmatrix} F_{uu}(U,V)U'P_{10} + F_{uv}(U,V)(U'Q_{10} + V'P_{10}) + F_{vv}(U,V)V'Q_{10} \\ G_{uu}(U,V)U'P_{10} + G_{uv}(U,V)(U'Q_{10} + V'P_{10}) + G_{vv}(U,V)V'Q_{10} \end{bmatrix} A_1$$

$$+ \begin{bmatrix} F_{uu}(U,V)(U')^2 + 2F_{uv}(U,V)U'V' + F_{vv}(U,V)(V')^2 \\ G_{uu}(U,V)(U')^2 + 2G_{uv}(U,V)U'V' + G_{vv}(U,V)(V')^2 \end{bmatrix} \frac{A_1^2}{2}$$

$$+ \begin{bmatrix} \hat{P}_{10}(\tau,\underset{\sim}{\xi},\theta) \\ \hat{Q}_{10}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} + \text{terms in } \exp(-\mu\theta),\ \exp(-2\mu\theta),$$

where $\hat{P}_{10}, \hat{Q}_{10}$ are known quantities, independent of A_1, B_1, and consisting of linear combinations of T-periodic functions of θ whose coefficients are polynomials in the $\underset{\sim}{\xi}$-derivatives of ϕ_0; in particular, if the $\underset{\sim}{\xi}$-derivatives of ϕ_0 go to 0 as $\tau\to+\infty$, then $\hat{P}_{10},\hat{Q}_{10}\to 0$ also. (This last property of $\hat{P}_{10}$ follows from property (IV.2.2b.4) of P_{10},Q_{10} and the fact that:

$$\hat{P}_{10} = \frac{1}{2}\left(F_{uu}P_{10}^2 + 2F_{uv}P_{10}Q_{10} + F_{vv}Q_{10}^2\right)\text{; similarly for } \hat{Q}_{10}.)$$

Before applying Lemma D to (2b), it should first be simplified by noticing the A_1^2-term can be eliminated. Since differentiating the equation for the limit cycle twice gives:

$$\begin{bmatrix} U''' \\ V''' \end{bmatrix} = \begin{bmatrix} F_u & F_v \\ G_u & G_v \end{bmatrix}\begin{bmatrix} U'' \\ V'' \end{bmatrix} + \begin{bmatrix} F_{uu}(U')^2 + 2F_{uv}U'V' + F_{vv}(V')^2 \\ G_{uu}(U')^2 + 2G_{uv}U'V' + G_{vv}(V')^2 \end{bmatrix},$$

we can rewrite (2b) as

$$\begin{bmatrix} (u_2 - \frac{1}{2}A_1^2U'')_\theta \\ (v_2 - \frac{1}{2}A_1^2U'')_\theta \end{bmatrix} = \begin{bmatrix} F_u & F_v \\ G_u & G_v \end{bmatrix}\begin{bmatrix} (u_2 - \frac{1}{2}A_1^2U'') \\ (v_2 - \frac{1}{2}A_1^2V'') \end{bmatrix} \tag{2c}$$

$$+\begin{bmatrix} -A_{1\tau}U' - \phi_{0\tau}A_1U'' + (1+\alpha)(\nabla^2A_1U' + (\nabla^2\phi_0A_1 + 2\nabla\phi_0\cdot\nabla A_1)U'' + |\nabla\phi_0|^2U''') \\ -A_{1\tau}V' - \phi_{0\tau}A_1V'' + (1-\alpha)(\nabla^2A_1V' + (\nabla^2\phi_0A_1 + 2\nabla\phi_0\cdot\nabla A_1)V'' + |\nabla\phi_0|^2V''') \end{bmatrix}$$

$$+\begin{bmatrix} F_{uu}U'P_{10} + F_{uv}(U'Q_{10} + V'P_{10}) + F_{vv}V'Q_{10} \\ G_{uu}U'P_{10} + G_{uv}(U'Q_{10} + V'P_{10}) + G_{vv}V'Q_{10} \end{bmatrix}$$

$$+\begin{bmatrix} \hat{P}_{10}(\tau,\underset{\sim}{\xi},\theta) \\ \hat{Q}_{10}(\tau,\underset{\sim}{\xi},\theta) \end{bmatrix} + \textit{terms in } \exp(-\mu\theta),\ \exp(-2\mu\theta).$$

In applying Lemma D to (2c), terms of $\mathcal{O}(\epsilon)$ will occur; these terms can be eliminated by a condition on A_1. To write this resulting equation, we use h_1, ℓ_1, m_1 from (5) and define:

$$\frac{1}{T}\int_0^T \begin{bmatrix} \hat{V}(s)U'''(s) - \hat{U}(s)V'''(s) \\ \hat{V}(s)U'''(s) + \hat{U}(s)V'''(s) \\ \hat{V}(F_{uu}U'P_{10}+F_{uv}(U'Q_{10}+V'P_{10})+F_{vv}V'Q_{10}) \\ \quad -\hat{U}(G_{uu}U'P_{10}+G_{uv}(U'Q_{10}+V'P_{10})+G_{vv}V'Q_{10}) \\ \hat{V}\hat{P}_{10} - \hat{U}\hat{Q}_{10} \end{bmatrix} \frac{ds}{U'\hat{V}-V'\hat{U}} = \begin{bmatrix} r_1 \\ s_1 \\ \hat{f}(\tau,\underset{\sim}{\xi}) \\ \hat{h}(\tau,\underset{\sim}{\xi}) \end{bmatrix}$$

The equation for A_1 is then:

$$A_{1\tau} = (1+\alpha h_1)\nabla^2 A_1 + 2(\ell_1+\alpha m_1)\nabla\phi_0\cdot\nabla A_1 \tag{4}$$
$$+ \left[\ell_1(-\phi_{0\tau}+\nabla^2\phi_0) + \alpha m_1\nabla^2\phi_0 + (r_1+\alpha s_1)|\nabla\phi_0|^2 + \hat{f}(\tau,\underset{\sim}{\xi})\right]A_1 + \hat{h}(\tau,\underset{\sim}{\xi}).$$

From (3) and the properties mentioned for P_{10}, Q_{10}, $\hat{P}_{10}$, $\hat{Q}_{10}$, we know $\hat{f},\hat{h}$ are polynomials in $\underset{\sim}{\xi}$-derivatives of $\phi_0(\tau,\underset{\sim}{\xi})$ and that $\hat{f},\hat{h}\to 0$ if the $\underset{\sim}{\xi}$-derivatives of ϕ_0 go to 0 as $\tau\to+\infty$.

BIBLIOGRAPHY

D. Aronson and H. Weinberger. Nonlinear diffusion in population genetics, combustion, and nerve propagation. Proceedings of the Tulane Program in Partial Differential Equations, Lecture Notes in Mathematics 446, Springer-Verlag, 1975.

A. D. Bazykin. Structural and dynamic stability of model prey- predator systems. Translation prepared in connection with the IIASA Workship on Computation of Stability Regions and Equilibria, July 1975, from "Volterra's system and the Michaelis-Menten Equations" (Russian) in Problem in Mathematical Genetics, V.A. Ratner (ed.), 1974, pp.103-142.

B. Belousov. Sb. ref. radiats. med. za. Medzig. Moscow, 1959.

G. Birkhoff and G.-C. Rota. Ordinary Differential Equations. Blaisdell, Watham, Mass., 1969.

J.A. Boa. Asymptotic calculation of a limit cycle. J. Math. Anal. Appl., 54(1976), pp.115-137.

J. Buck and E. Buck. Synchronous fireflies. Sci. Amer., 234(1976), pp.74-85.

B. Carnahan, H. A. Luther, and J. O. Wilkes. Applied Numerical Methods. Wiley, New York, 1969.

G. Carpenter. Traveling wave solutions of nerve inpulse equations. Ph.D. Thesis, University of Wisconsin, Madison, Wisconsin, 1974.

G. F. Carrier and C. E. Pearson. Partial Differential Equations. Academic Press, New York, 1976.

R. G. Casten, H. Cohen, and P. A. Lagerstrom. Perturbation analysis of an approximation to the Hodgkin-Huxley theory. Quart. Appl. Math., 32(1975), pp.365-402.

K. N. Chueh, C. C. Conley, and J. A. Smoller. Positively invariant regions for systems of nonlinear diffusion equations. Ind. Univ. Math. Jour., 26(1977), pp.373-392.

E. A. Coddington and N. Levinson. Theory of Ordinary Differential Equations. McGraw-Hill, New York, 1955.

H. Cohen. Nonlinear diffusion problems. Studies in Applied Mathematics, A. H. Taub (ed.), Prentice-Hall, Englewood Cliffs, N.J., 1971.

D. S. Cohen. Multiple solutions and periodic oscillations in nonlinear diffusion processes. SIAM J. Appl. Math., 25(1973), pp.640-654.

D. S. Cohen, F. C. Hoppensteadt, and R. M. Miura. Slowly modulated oscillations in nonlinear diffusion processes. SIAM J. Appl. Math., 33(1977), pp.217-229.

D. S. Cohen, J. C. Neu, and R. Rosales. Rotating spiral wave solutions of reaction-diffusion equations. SIAM J. Appl. Math., 35(1978), pp.536-547.

D. S. Cohen and S. Rosenblatt. Multi-species interaction with hereditary effects and spatial diffusion. Preprint, 1978?

E. Conway, D. Hoff, and J. Smoller. Large time behavior of solutions of systems of nonlinear reaction-diffusion equations. SIAM J. Appl. Math., 35(1978), pp.1-16.

E. D. Conway and J. A. Smoller. A comparison technique for systems of reaction-diffusion equations. Comm. in Part. Diff. Eqns., 2(1977), pp.679-697.

D. Cope. Reaction-diffusion systems with explicit traveling wave and transient solutions. SIAM J. Appl. Math., 37(1979), pp.316-324.

D. Cope. Stability of limit cycle solutions of reaction-diffusion equations. SIAM J. Appl. Math., to appear 1980.

R. Courant and D. Hilbert. Methods of Mathematical Physics. Vol.I., Wiley (Interscience), New York, 1953.

F. H. Crick and P. A. Lawrence. Compartments and polyclones in insect development. Science, 189(1975), pp.340-347.

J. Cronin. Some mathematics of biological oscillations. SIAM Rev., 19(1977), pp.100-138.

S. P. Diliberto. On systems of ordinary differential equations. Contributions to the Theory of Nonlinear Oscillations, S. Lefschetz (ed.), Princeton Univ. Press, Princeton, 1950.

M. S. P. Eastham. The Spectral Theory of Periodic Differential Equations. Scottish Academic Press, Edinburgh, 1973.

J. W. Evans. Nerve axon equations: I Linear approximations. Ind. Univ. Math. J., 21(1972), pp.877-885.

J. W. Evans. Nerve axon equations: II Stability at rest. Ind. Univ. Math. J., 22(1972), pp.75-90.

J. W. Evans. Nerve axon equations: III Stability of the nerve impulse. Ind. Univ. Math. J., 22(1972), pp.577-593.

J. W. Evans. Nerve axon equations: IV The stable and the unstable impulse. Ind. Univ. Math. J., 24(1975), pp.1169-1190.

J. W. Evans and J. Feroe. Local stability theory of the nerve impulse. Preprint, 1977?

J. Evans and N. Shenk. Solutions to axon equations. Biophys. J., 10(1970), pp.1090-1101.

M. A. Evgrafov. Analytic Functions. Dover, New York, 1978.

N. Fenichel. Asymptotic stability with rate conditions. Ind. Univ. Math. J., 23(1974), pp.1109-1137.

N. Fenichel. Asymptotic stability with rate conditions, II. Ind. Univ. Math. J., 26(1977), pp.81-93.

E. Fermi. Thermodynamics. Dover, New York, 1956.

R. J. Field and R. M. Noyes. Oscillations in chemical systems. IV: Limit cycle behavior in a model of a real chemical reaction. J. Chem. Phys., 160(1974), pp.1877-1884.

P. C. Fife. Stationary patterns for reaction-diffusion equations. Technical Report 1709, Mathematics Research Center, University of Wisconsin, Madison, 1977.

P. C. Fife. Results and open questions in the asymptotic theory of reaction-diffusion equations. Nonlinear Evolution Equations, M. G. Crandall (ed.), Academic Press, New York, 1978.

P. C. Fife. Asymptotic states for equations of reaction and diffusion. Bull. Amer. Math. Soc., (1978).

P. C. Fife. Mathematical Aspects of Reacting and Diffusing Systems. Lecture Notes in Biomathematics, Vol. 28, Springer-Verlag, New York, 1979.

P. C. Fife and J. B. McLeod. The approach of solutions of nonlinear diffusion equations to traveling wave solutions. Bull. Amer. Math. Soc., 81(1975), pp.1075-1078. Appears in full in Arch. Rat. Mech. Anal., 65(1977), pp.335-361.

W. E. Fitzgibbon and H.F. Walker (eds.). Nonlinear Diffusion. Pitman, London, 1977.

R. Fitzhugh. Thresholds and plateaus in the Hodgkin-Huxley nerve equations. J. Gen. Physiol., 43(1960), pp.867-896.

R. Fitzhugh. Impulses and physiological states in theoretical models of nerve membrane. Biophys. J., 1(1961), pp.445-466.

R. Fitzhugh. Mathematical models of excitation and propagation in nerve. Biological Engineering, H.P. Schwan (ed.), McGraw-Hill, New York, 1969.

L. Flatto and N. Levinson. Periodic solutions of singularly perturbed systems. J. Rat. Mech. Anal., 4(1955), pp.943-950.

B. Fornberg. On the instability of leapfrog and Crank-Nicolson approximations of a nonlinear partial differential equation. Math. Comp., 27(1973), pp.45-57.

K. O. Friedrichs and W. R. Wasow. Singular perturbations of nonlinear oscillations. Duke Math. Jour., 13(1946), pp.367-381.

A. Garcia-Bellido, P. A. Lawrence, and G. Morata. Compartments in animal development. Sci. Amer., 241(1979), pp.102-110.

J. M. Greenberg. Periodic solutions to reaction-diffusion equations. SIAM J. Appl. Math., 30(1976), pp.199-205.

J. M. Greenberg. Axi-symmetric, time-periodic solutions of reaction-diffusion equations. SIAM J. Appl. Math., 34(1978), pp.391-397.

J. Guckenheimer. Isochrons and phaseless sets. J. Math. Biol., 1(1975), pp.259-273.

A. Halanay. Differential equations. Academic Press, New York, 1966.

S. P. Hastings. The existence of periodic solutions to Nagumo's equation. Quart. J. Math. Oxford, 25(1974), pp.369-378.

S. P. Hastings. Some mathematical problems from neurobiology. Amer. Math. Monthly, 82(1975), pp.881-894.

S. P. Hastings. On the existence of homoclinic and periodic orbits for the Fitzhugh-Nagumo equations. Quart. J. Math. Oxford, 27(1976), pp.123-134.

S. P. Hastings. On the traveling wave solutions of the Hodgkin-Huxley equations. Arch. Rat. Mech. and Anal., 60(1976), pp.229-257.

S. P. Hastings and J. D. Murray. The existence of oscillatory solutions in the Field-Noyes model for the Belousov-Zhabotinskii reaction. SIAM J. Appl. Math., 28(1975), pp.678-688.

J. Hiernaux and T. Erneux. Chemical patterns in circular morphogenetic fields. Bull. Math. Biol., 41(1979), pp.461-468.

A. L. Hodgkin and A. F. Huxley. A quantitative description of membrane current and its application to conduction and excitation in nerves. J. Physiol., 117(1952), pp.500-544.

E. Hopf. Abzweigung einer periodischen Lösung von einer stationären Lösung eines Differential-systems. Ber. Math.-Phys. Kl. Sächs. Acad. Wiss. Leipzig, 94(1942), pp.1-22. Translated in Marsden and McCracken, op.cit.

L. R. Howard and Nancy Kopell. Slowly varying waves and shock structures in reaction-diffusion equations. Stud. in Appl. Math., 56(1977), pp.94-145.

G. J. Kasparek and T. C. Bruice. Observations on an oscillating reaction. The reaction of potassium bromate, ceric sulfate, and a dicarboxylic acid. Inorg. Chem., 10(1971), pp.382-388.

S. A. Kaufman, R. M. Shymko, and K. Trabert. Control of sequential compartment formation in Drosophila. Science, 199(1978), pp.259-270.

E. F. Keller and L. A. Segel. Initiation of slime mold aggregation viewed as an instability. J. Theor. Biol., 26(1970), pp.399-415.

E. F. Keller and L. A. Segel. Model for chemotaxis. J. Theor. Biol., 30(1971), pp.225-234.

E. F. Keller and L. A. Segel. Traveling bands of chemotactic bacteria: a theoretical analysis. J. Theor. Biol., 30(1971), pp.235-248.

A. Kolmogorov, I. Petrovsky, and N. Piskunov. Étude de l'équation de la chaleur avec croissance et son application à un probleme biologique. Bull. Univ. État Moscow, 6(1937), pp.1-25.

N. Kopell and L. N. Howard. Plane wave solutions to reaction-diffusion equations. Stud. Appl. Math., 52(1973), pp.291-328.

Y. Kuramoto and T. Yamada. Pattern formation in oscillatory chemical reactions. Prog. Th. Phys., 56(1976), pp. 724-740.

B. Lavenda, G. Nicolis, and M. Herschkowitz-Kaufman. Chemical instabilities and relaxation oscillations. J. Theor. Biol., 32(1971), pp.283-292.

M. Lees. An extrapolated Crank-Nicolson difference scheme for quasilinear parabolic equations. Numerical Solution of Partial Differential Equations, W. F. Ames (ed.), Barnes and Noble, New York, 1969.

S. Lefschetz. Differential Equations: Geometric Theory. Dover, New York, 1977.

A. J. Lotka. Elements of Mathematical Biology. Dover, New York, 1956.

J. E. Marsden and M. McCracken. The Hopf Bifurcation and its Applications. Springer-Verlag, New York, 1976.

H. J. K. Moet. A note on the asymptotic behavior of solutions of the KPP equation. SIAM J. Math. Anal., 10(1979), pp.728-732.

J. Nagumo, S. Arimoto, and S. Yoshizawa. An active pulse transmission line simulating nerve axon. Proc. IRE, 50(1962), pp.2061-2070.

J. C. Neu. Chemical waves and the diffusive coupling of limit cycle oscillators. SIAM J. Appl. Math., 36(1979), pp.509-515.

R. M. Noyes, R. J. Field, and E. Körös. Oscillations in chemical systems. I. Detailed mechanism in a system showing temporal oscillations. J. Amer. Chem. Soc., 94(1972), pp.1394-1395.

R. M. Noyes, R. J. Field, and E. Körös. Oscillations in chemical systems. II. Thorough analysis of temporal oscillation in the bromate-cerium-malonic acid system. J. Amer. Chem. Soc., 94(1972), pp.8649-8664.

P. Ortoleva and J. Ross. Phase waves in oscillatory chemical reactions. J. Chem. Phys., 58(1973), pp.5673-5680.

P. Ortoleva and J. Ross. On a variety of wave phenomena in chemical reactions. J. Chem. Phys., 60(1974), pp.5090-5107.

H. G. Othmer. Current problems in pattern formation. Lectures on Mathematics in the Life Sciences, S. A. Levin (ed.), Amer. Math. Soc., 9(1977), pp.57-85.

H. G. Othmer and L. A. Scriven. Interactions of reaction and diffusion in open systems. Ind. Eng. Chem. Fund., 8(1969), pp.302-313.

I. Prigogine and R. Lefever. Symmetry breaking instabilities in dissipative systems. II. J. Chem. Phys., 48(1968), pp.1695-1700.

I. Prigogine, R. Lefever, A. Goldbeter, and M. Herschkowitz-Kaufman. Symmetry breaking instabilities in biological systems. Nature, 223(1969), pp.913-916.

I. Prigogine and G. Nicolis. On symmetry-breaking instabilities in dissipative systems. J. Chem. Phys., 46(1967), pp.3542-3550.

M. H. Protter and H. F. Weinberger. Maximum Principles in Differential Equations. Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1967.

R. D. Richtmeyer and K. W. Morton. Difference Methods for Initial Value Problems. Wiley (Interscience), New York, 1967.

J. Rinzel. Repetitive Nerve Impulse Propagation: Numerical Results and Methods. In Fitzgibbon and Walker, op.cit.

J. Rinzel and J. Keller. Traveling wave solutions of a nerve conduction equation. Biophys. J., 13(1973), pp.1313-1337.

G. Rosen. Necessary condition for the existence of periodic solutions to systems of reaction-diffusion equations. Math. Biosc., 21(1974), pp.345-350.

D. H. Sattinger. On the stability of waves of nonlinear parabolic systems. Adv. in Math., 22(1976), pp.312-355.

D. H. Sattinger. Weighted norms for the stability of traveling waves. J. Diff. Eqns., 25(1977), pp.130-144.

M. E. Solomon. Population Dynamics. Studies in Biology No.18, Edward Arnold (Publishers) Ltd., London, 1969.

A. M. Turing. The chemical basis of morphogenesis. Phil. Trans. Roy, Soc. B, 237(1952), pp.37-72.

J. J. Tyson. Some further studies of nonlinear oscillations in chemical systems. J. Chem. Phys., 58(1973), pp.3919-3930.

J. Tyson and S. Kaufman. Control of mitosis by a continuous biochemical oscillation: synchronization; spacially inhomogeneous oscillations. J. Math. Biol., (1975), pp.289-310.

J. J. Tyson and J. C. Light. Properties of bimolecular and trimolecular chemical reaction systems. J. Chem. Phys., 59(1973), pp.4164-4173.

J. Varah. Stability restrictions on second order, three level finite difference schemes for parabolic differential equations. Technical Report 78-9, Department of Computer Science, University of British Columbia, Vancouver, 1978.

J. Walker. The amateur scientist: chemical systems that oscillate between one color and another. Sci. Amer., 239(1978), pp.152-160.

W. Wasow. Asymptotic Expansions for Ordinary Differential Equations. R. E. Kriegar, Huntington, New York, 1976.

A. T. Winfree. Spiral waves of chemical activity. Science, 175(1972), pp.634-636.

A. T. Winfree, Rotating reactions, Sci. Amer., 230(1974), pp.82-95.

A. T. Winfree, Patterns of phase compromise in biological cycles. J. Math. Biol., 1(1974), pp.73-95.

A. T. Winfree. 24 hard problems about the mathematics of 24 hour rhythmns. Manuscript of talk presented at AMS-SIAM Summer Seminar on Nonlinear Oscillations in Biology, Salt Lake City, 1978.

T. Yamada and Y. Kuramoto. Spiral waves in a nonlinear dissipative system.' Prog. Th. Phys., 55(1976), pp.2035-2036.

A. N. Zaikin and A. M. Zhabotinskii. Concentration wave propagation in two-dimensional liquid-phase self-oscillating system. Nature, 225(1976), pp.535-537.

CNA Professional Papers — 1976 to Present*

PP 141
Mizrahi, Maurice M., "Generalized Hermite Polynomials,"* 5 pp., Feb 1976 (Reprinted from the Journal of Computational and Applied Mathematics, Vol. 1, No. 4 (1975), 273-277).
*Research supported by the National Science Foundation

PP 143
Horowitz, Stanley and Sherman, Allan (LCdr., USN), "Maintenance Personnel Effectiveness in the Navy," 33 pp., Jan 1976 (Presented at the RAND Conference on Defense Manpower, Feb 1976) AD A021 581

PP 144
Durch, William J., "The Navy of the Republic of China – History, Problems, and Prospects," 66 pp., Aug 1976 (Published in "A Guide to Asiatic Fleets," ed. by Barry M. Blechman and Robert Berman, Naval Institute Press) AD A030 460

PP 145
Kelly, Anne M., "Port Visits and the "Internationalist Mission" of the Soviet Navy," 36 pp., Apr 1976, AD A023 436

PP 147
Kessler, J. Christian, "Legal Issues in Protecting Offshore Structures," 33 pp., Jun 1976 (Prepared under task order N00014-68-A-0091-0023 for ONR) AD A028 389

PP 149
Squires, Michael L., "Counterforce Effectiveness: A Comparison of the Tsipis "K" Measure and a Computer Simulation," 24 pp., Mar 1976 (Presented at the International Study Association Meetings, 27 Feb 1976) AD A022 591

PP 150
Kelly, Anne M. and Petersen, Charles, "Recent Changes in Soviet Naval Policy: Prospects for Arms Limitations in the Mediterranean and Indian Ocean," 28 pp., Apr 1976, AD A 023 723

PP 151
Horowitz, Stanley A., "The Economic Consequences of Political Philosophy," 8 pp., Apr 1976 (Reprinted from Economic Inquiry, Vol. XIV, No. 1, Mar 1976)

PP 152
Mizrahi, Maurice M., "On Path Integral Solutions of the Schrodinger Equation, Without Limiting Procedure,"* 10 pp., Apr 1976 (Reprinted from Journal of Mathematical Physics, Vol. 17, No. 4 (Apr 1976), 566-575).
*Research supported by the National Science Foundation

PP 153
Mizrahi, Maurice M., "WKB Expansions by Path Integrals, With Applications to the Anharmonic Oscillator,"* 137 pp., May 1976, AD A025 440
*Research supported by the National Science Foundation

PP 154
Mizrahi, Maurice M., "On the Semi-Classical Expansion in Quantum Mechanics for Arbitrary Hamiltonians," 19 pp., May 1976 (Published in Journal of Mathematical Physics, Vol. 18, No. 4, pp. 786-790, Apr 1977), AD A025 441

PP 155
Squires, Michael L., "Soviet Foreign Policy and Third World Nations," 26 pp., Jun 1976 (Prepared for presentation at the Midwest Political Science Association meetings, Apr 30, 1976) AD A028 388

PP 156
Stallings, William, "Approaches to Chinese Character Recognition," 12 pp., Jun 1976 (Reprinted from Pattern Recognition (Pergamon Press), Vol. 8, pp. 87-98, 1976) AD A028 692

PP 157
Morgan, William F., "Unemployment and the Pentagon Budget: Is There Anything in the Empty Pork Barrel?" 20 pp., Aug 1976 AD A030 455

PP 158
Haskell, LCdr. Richard D. (USN), "Experimental Validation of Probability Predictions," 25 pp., Aug 1976 (Presented at the Military Operations Research Society Meeting, Fall 1976) AD A030 458

PP 159
McConnell, James M., "The Gorshkov Articles, The New Gorshkov Book and Their Relation to Policy," 93 pp., Jul 1976 (Published in Soviet Naval Influence: Domestic and Foreign Dimensions, ed. by M. MccGwire and J. McDonnell; New York; Praeger, 1977) AD A029 227

PP 160
Wilson, Desmond P., Jr., "The U.S. Sixth Fleet and the Conventional Defense of Europe," 50 pp., Sep 1976, AD A030 457

PP 161
Melich, Michael E. and Peet, Vice Adm. Ray (USN, Retired), "Fleet Commanders: Afloat or Ashore?" 9 pp., Aug 1976 (Reprinted from U.S. Naval Institute Proceedings, Jun 1976) AD A030 456

PP 162
Friedheim, Robert L., "Parliamentary Diplomacy," 106 pp. Sep 1976 AD A033 306

PP 163
Lockman, Robert F., "A Model for Predicting Recruit Losses," 9 pp., Sep 1976 (Presented at the 84th annual convention of the American Psychological Association, Washington, D.C., 4 Sep 1976) (Published in Defense Manpower Policy (Richard V. L. Cooper, ed.), The Rand Corporation, 1979), AD A030 459

PP 164
Mahoney, Robert B., Jr., "An Assessment of Public and Elite Perceptions in France, The United Kingdom, and the Federal Republic of Germany," 31 pp., Feb 1977 (Presented at Conference "Perception of the U.S. – Soviet Balance and the Political Uses of Military Power" sponsored by Director, Advanced Research Projects Agency, April 1976) AD A036 599

PP 165
Jondrow, James M. "Effects of Trade Restrictions on Imports of Steel," 67 pp., November 1976, (Delivered at ILAB Conference in Dec 1976)

PP 166 – Revised
Feldman, Paul, "Why It's Difficult to Change Regulation," Oct 1976, AD A037 682

PP 167
Kleinman, Samuel, "ROTC Service Commitments: a Comment," 4 pp., Nov 1976, (Published in Public Choice, Vol. XXIV, Fall 1976) AD A033 305

PP 168
Lockman, Robert F., "Revalidation of CNA Support Personnel Selection Measures," 36 pp., Nov 1976

PP 169
Jacobson, Louis S., "Earnings Losses of Workers Displaced from Manufacturing Industries," 38 pp., Nov 1976, (Delivered at ILAB Conference in Dec 1976), AD A039 809

PP 170
Brechling, Frank P., "A Time Series Analysis of Labor Turnover," Nov 1976. (Delivered at ILAB Conference in Dec 1976)

PP 171
Jordan, A. S.* and Ralston, J. M., "A Diffusion Model for GaP Red LED Degradation," 10 pp., Nov 1976, (Published in Journal of Applied Physics, Vol. 47, pp. 4518-4527, Oct 1976)
*Bell Laboratories

PP 172
Classen, Kathleen P., "Unemployment Insurance and the Length of Unemployment," Dec 1976, (Presented at the University of Rochester Labor Workshop on 16 Nov 1976)

PP 173
Kleinman, Samuel D., "A Note on Racial Differences in the Added-Worker/Discouraged-Worker Controversy," 2 pp., Dec 1976, (Published in the American Economist, Vol. XX, No. 1, Spring 1976)

PP 174
Mahoney, Robert B., Jr., "A Comparison of the Brookings and International Incidents Projects," 12 pp. Feb 1977 AD A037 206

PP 175
Levine, Daniel; Stoloff, Peter and Spruill, Nancy, "Public Drug Treatment and Addict Crime," June 1976, (Published in Journal of Legal Studies, Vol 5, No. 2)

PP 176
Felix, Wendi, "Correlates of Retention and Promotion for USNA Graduates," 38 pp., Mar 1977, AD A039 040

PP 177
Lockman, Robert F. and Warner, John T. "Predicting Attrition: A Test of Alternative Approaches," 33 pp. Mar 1977. (Presented at the OSD/ONR Conference on Enlisted Attrition, Xerox International Training Center, Leesburg, Virginia, 4-7 April 1977), AD A039 047

PP 178
Kleinman, Samuel D., "An Evaluation of Navy Unrestricted Line Officer Accession Programs," 23 pp. April 1977, (Presented at the NATO Conference on Manpower Planning and Organization Design, Stresa, Italy, 20 June 1977), AD A039 048

***CNA Professional Papers with an AD number may be obtained from the National Technical Information Service, U.S. Department of Commerce, Springfield, Virginia 22151. Other papers are available from the Management Information Office, Center for Naval Analyses, 2000 North Beauregard Street, Alexandria, Virginia 22311. An Index of Selected Publications is also available on request. The index includes a Listing of Professional Papers, with abstracts, issued from 1969 to February 1978.**

PP 179
Stoloff, Peter H. and Balut, Stephen J., "Vacate: A Model for Personnel Inventory Planning Under Changing Management Policy," 14 pp. April 1977, (Presented at the NATO Conference on Manpower *Planning and Organization Design, Stresa*, Italy, 20 June 1977), AD A039 049

PP 180
Horowitz, Stanley A. and Sherman, Allan, "The Characteristics of Naval Personnel and Personnel Performance," 16 pp. April 1977, (Presented at the NATO Conference on Manpower Planning and Organization Design, Stresa, Italy, 20 June 1977), AD A039 050

PP 181
Balut, Stephen J. and Stoloff, Peter, "An Inventory Planning Model for Navy Enlisted Personnel," 35 pp., May 1977 (Prepared for presentation at the Joint National Meeting of the Operations Research Society of America and The Institute for Management Science. 9 May 1977, San Francisco, California), AD A042 221

PP 182
Murray, Russell, 2nd, "*The Quest for the Perfect* Study or My First 1138 Days at CNA," 57 pp., April 1977

PP 183
Kassing, David, "Changes in Soviet Naval Forces," 33 pp., November, 1976, (Published as part of Chapter 3, "General Purpose Forces: Navy and *Marine Corps*," in Arms, Men, and Military Budgets, Francis P. Hoeber and William Schneider, Jr. (eds.), (Crane, Russak & Company, Inc. New York), 1977), AD A040 106

PP 184
Lockman, Robert F., "An Overview of the OSD/ONR Conference on First Term Enlisted Attrition," 22 pp., June 1977, (Presented to the 39th MORS Working Group on Manpower and Personnel Planning, Annapolis, Md., 23-30 Jun 1977), AD A043 618

PP 185
Kassing, David, "New Technology and Naval Forces in the South Atlantic," 22 pp. (This paper was the basis for a presentation made at the Institute for Foreign Policy Analyses, Cambridge, Mass., 28 April 1977), AD A043 619

PP 186
Mizrahi Maurice M., "Phase Space Integrals, Without Limiting Procedure," 31 pp., May 1977, (Invited paper presented at the 1977 NATO Institute on Path Integrals and Their Application in Quantum *Statistical, and Solid State Physics*, Antwerp, Belgium, July 17-30, 1977) (Published in Journal of Mathematical Physics 19(1), pp 298-307, Jan 1978), AD A040 107

PP 187
Coile, Russell C. "Nomography for Operations Research," 35 pp. April 1977 (Presented at the Joint *National Meeting* of the Operations Research Society of America and The Institute for Management Services, San Francisco, California, 9 May 1977), AD A043 620

PP 188
Durch, William J., "Information Processing and Outcome Forecasting for Multilateral Negotiations: Testing One Approach," 53 pp. May 1977 (Prepared for presentation to the 18th Annual Convention of the International Studies Association, Chase Park Plaza Hotel, St. Louis, Missouri, March 16-20, 1977), AD A042 222

PP 189
Coile, Russell C., "Error Detection in Computerized Information Retrieval Data Bases," July, 1977, 13 pp. (Presented at the Sixth Cranfield International Conference on Mechanized Information Storage and Retrieval Systems, Cranfield Institute of Technology, Cranfield, Bedford, England, 26-29 July 1977), AD A043 580

PP 190
Mahoney, Robert B., Jr., "European Perceptions and East-West Competition," 96 pp., July 1977 (Prepared for presentation at the annual meeting of the International Studies Association, St. Louis, Mo., March, 1977), AD A043 661

PP 191
Sawyer, Ronald, "The Independent Field Assignment: One Man's View," August 1977, 25 pp.

PP 192
Holen, Arlene, "Effects of Unemployment Insurance Entitlement on Duration and Job Search Outcome," August 1977, 6 pp., (Reprinted from Industrial and Labor Relations Review, Vol., 30, No. 4, Jul 1977)

PP 193
Horowitz, Stanley A., "A Model of Unemployment Insurance and the Work Test," August 1977, 7 pp. (*Reprinted from Industrial and Labor Relations* Review, Vol. 30, No. 40, Jul 1977)

PP 194
Classen, Kathleen P., "The Effects of Unemployment Insurance on the Duration of Unemployment and Subsequent Earnings," August 1977, 7 pp. (Reprinted from Industrial and Labor Relations *Review*, Vol. 30, No. 40, Jul 1977)

PP 195
Brechling, Frank, "Unemployment Insurance Taxes and Labor Turnover: Summary of Theoretical Findings," 12 pp. (Reprinted from Industrial and Labor Relations Review, Vol. 30, No. 40, Jul 1977)

PP 196
Ralston, J. M. and Lorimor, O. G., "Degradation of Bulk Electroluminescent Efficiency in Zn, O-Doped GaP LED's," July 1977, 3 pp. (Reprinted from IEEE Transactions on Electron Devices, Vol ED-24, No. 7, July 1977)

PP 197
Wells, Anthony R., "The Centre for Naval Analyses," 14 pp., Dec 1977, AD A049 107

PP 198
Classen, Kathleen P., "The Distributional Effects of *Unemployment Insurance*," 25 *pp., Sept.* 1977 (Presented at a Hoover Institution Conference on Income Distribution, Oct 7-8, 1977), AD A054 423

PP 199
Durch, William J., "Revolution From A F.A.R. – The Cuban Armed Forces in Africa and the Middle East," Sep 1977, 16 pp., AD A046 268

PP 200
Powers, Bruce F., "The United States Navy," 40 pp. Dec 1977 (Published as a chapter in The U.S. War Machine by Salamander Books, England, 1978), AD A049 108

PP 201
Durch, William J., "The Cuban Military in Africa and The Middle East: From Algeria to Angola," Sep 1977, 67 pp., AD A045 675

PP 202
Feldman, Paul, "Why Regulation Doesn't Work," (Reprinted from Technological Change and Welfare in the Regulated Industries, Brookings Reprint 219, 1971, and Review of Social Economy, Vol. XXIX, March, 1971, No. 1.) Sep 1977, 8 pp

PP 203
Feldman, Paul, "Efficiency, Distribution, and the Role of Government in a Market Economy," (Reprinted from The Journal of Political Economy, Vol. 79, No. 3, May/June 1971.) Sep 1977, 19 pp., AD A045 675

PP 204
Wells, Anthony R., "The 1967 June War: Soviet Naval Diplomacy and The Sixth Fleet – A Reappraisal," Oct 1977, 36 pp., AD A047 236

PP 205
Coile, Russell C., "A Bibliometric Examination of the Square Root Theory of Scientific Publication *Productivity*," (*Presented at the annual meeting of* the American Society for Information Science, Chicago, Illinois, 29 September 1977.) Oct 1977, 6 pp., AD A047 237

PP 206
McConnell, James M., "Strategy and Missions of the Soviet Navy in the Year 2000," 48 pp., Nov 1977 (Presented at a Conference on Problems of Sea Power as we Approach the 21st Century, sponsored by the American Enterprise Institute for Public Policy Research, 6 October 1977, and subsequently published in a collection of papers by the Institute), AD A047 244

PP 207
Goldberg, Lawrence, "Cost-Effectiveness of Potential Federal Policies *Affecting Research &* Development Expenditures in the Auto, Steel and Food Industries," 36 pp., Oct 1977, (Presented at Southern Economic Association Meetings beginning 2 November 1977), AD A046 269

PP 208
Roberts, Stephen S., "The Decline of the Overseas Station Fleets: The United States Asiatic Fleet and the Shanghai Crisis, 1932," 18 pp., Nov 1977 (Reprinted from The American Neptune, Vol. XXXVII, No. 3, July 1977), AD A047 245

PP 209 – Classified.

PP 210
Kassing, David, "Protecting The Fleet," 40 pp., Dec 1977 (Prepared for the American Enterprise Institute Conference on Problems of Sea Power as We Approach the 21st Century, October 6-7, 1977), AD A049 109

PP 211
Mizrahi, Maurice M., "On Approximating the Circular Coverage Function," 14 pp., Feb 1978, AD A054 429

PP 212
Mangel, Marc, "On Singular Characteristic Initial Value Problems with Unique Solutions," 20 pp., Jun 1978, AD A058 535

PP 213
Mangel, Marc, "Fluctuations in Systems with Multiple Steady States. Application to Lanchester Equations," 12 pp., Feb 78, (Presented at the First Annual Workshop on the Information Linkage Between Applied Mathematics and Industry, Naval PG School, Feb 23-25, 1978), AD A071 472

PP 214
Weinland, Robert G., "A Somewhat Different View of The Optimal Naval Posture," 37 pp., Jun 1978 (Presented at the 1976 Convention of the American Political Science Association (APSA/IUS Panel on "Changing Strategic Requirements and Military Posture"), Chicago, Ill., September 2, 1976), AD A056 228

PP 215
Coile, Russell C., "Comments on: Principles of Information Retrieval by Manfred Kochen," 10 pp., Mar 78, (Published as a Letter to the Editor, Journal of Documentation, Vol. 31, No. 4, pages 298-301, December 1975), AD A054 426

PP 216
Coile, Russell C., "Lotka's Frequency Distribution of Scientific Productivity," 18 pp., Feb 1978, (Published in the Journal of the American Society for Information Science, Vol. 28, No. 6, pp. 366-370, November 1977), AD A054 425

PP 217
Coile, Russell C., "Bibliometric Studies of Scientific Productivity," 17 pp., Mar 78, (Presented at the Annual meeting of the American Society for Information Science held in San Francisco, California, October 1976), AD A054 442

PP 218 – Classified.

PP 219
Huntzinger, R. LaVar, "Market Analysis with Rational Expectations: Theory and Estimation," 60 pp., Apr 78, AD A054 422

PP 220
Maurer, Donald E., "Diagonalization by Group Matrices," 26 pp., Apr 78, AD A054 443

PP 221
Weinland, Robert G., "Superpower Naval Diplomacy in the October 1973 Arab-Israeli War," 76 pp., Jun 1978 (Published in Seapower in the Mediterranean: Political Utility and Military Constraints, The Washington Papers No. 61, Beverly Hills and London: Sage Publications, 1979) AD A055 564

PP 222
Mizrahi, Maurice M., "Correspondence Rules and Path Integrals," 30 pp., Jun 1978 (Invited paper presented at the CNRS meeting on "Mathematical Problems in Feynman's Path Integrals," Marseille, France, May 22-26, 1978) (Published in Springer Verlag Lecture Notes in Physics, 106, (1979) 234-253) AD A055 536

PP 223
Mangel, Marc, "Stochastic Mechanics of Molecule-Ion Molecule Reactions," 21 pp., Jun 1978, AD A056 227

PP 224
Mangel, Marc, "Aggregation, Bifurcation, and Extinction in Exploited Animal Populations*," 48 pp., Mar 1978, AD A058 536
*Portions of this work were started at the Institute of Applied Mathematics and Statistics, University of British Columbia, Vancouver, B.C., Canada

PP 225
Mangel, Marc, "Oscillations, Fluctuations, and the Hopf Bifurcation*," 43 pp., Jun 1978, AD A058 537
*Portions of this work were completed at the Institute of Applied Mathematics and Statistics, University of British Columbia, Vancouver, Canada

PP 226
Ralston, J. M. and J. W. Mann*, "Temperature and Current Dependence of Degradation in Red Emitting GaP LEDs," 34 pp., Jun 1978 (Published in Journal of Applied Physics, 50, 3630, May 1979) AD A058 538
*Bell Telephone Laboratories, Inc.

PP 227
Mangel, Marc, "Uniform Treatment of Fluctuations at Critical Points," 50 pp., May 1978, AD A058 539

PP 228
Mangel, Marc, "Relaxation at Critical Points: Deterministic and Stochastic Theory," 54 pp., Jun 1978, AD A058 540

PP 229
Mangel, Marc, "Diffusion Theory of Reaction Rates, I: Formulation and Einstein-Smoluchowski Approximation," 50 pp., Jan 1978, AD A058 541

PP 230
Mangel, Marc, "Diffusion Theory of Reaction Rates, II Ornstein-Uhlenbeck Approximation," 34 pp., Feb 1978, AD A058 542

PP 231
Wilson, Desmond P., Jr., "Naval Projection Forces: The Case for a Responsive MAF," Aug 1978, AD A058 543

PP 232
Jacobson, Louis, "Can Policy Changes Be Made Acceptable to Labor?" Aug 1978 (Submitted for publication in Industrial and Labor Relations Review), AD A061 528

PP 233
Jacobson, Louis, "An Alternative Explanation of the Cyclical Pattern of Quites," 23 pp., Sep 1978

PP 234 – Revised
Jondrow, James and Levy, Robert A., "Does Federal Expenditure Displace State and Local Expenditure: The Case of Construction Grants," 25 pp., Oct 1979, AD A061 529

PP 235
Mizrahi, Maurice M., "The Semiclassical Expansion of the Anharmonic-Oscillator Propagator," 41 pp., Oct 1978 (Published in Journal of Mathematical Physics 20 (1979), pp. 844-855), AD A061 538

PP 237
Maurer, Donald, "A Matrix Criterion for Normal Integral Bases," 10 pp., Jan 1979 (Published in the Illinois Journal of Mathematics, Vol. 22 (1978), pp. 672-681

PP 238
Utgoff, Kathleen Classen, "Unemployment Insurance and The Employment Rate," 20 pp., Oct 1978 (Presented at the Conference on Economic Indicators and Performance: The Current Dilemma Facing Government and Business Leaders, presented by Indiana University Graduate School of Business), AD A061 527

PP 239
Trost, R. P. and Warner, J. T., "The Effects of Military Occupational Training on Civilian Earnings: An Income Selectivity Approach," 38 pp., Nov 1979, AD A077 831

PP 240
Powers, Bruce, "Goals of the Center for Naval Analyses," 13 pp., Dec 1978, AD A063 759

PP 241
Mangel, Marc, "Fluctuations at Chemical Instabilities," 24 pp., Dec 1978 (Published in Journal of Chemical Physics, Vol. 69, No. 8, Oct 15, 1978), AD A063 787

PP 242
Simpson, William R., "The Analysis of Dynamically Interactive Systems (Air Combat by the Numbers)" 160 pp., Dec 1978, AD A063 760

PP 243
Simpson, William R., "A Probabilistic Formulation of Murphy Dynamics as Applied to the Analysis of Operational Research Problems," 18 pp., Dec 1978, AD A063 761

PP 244
Sherman, Allan and Horowitz, Stanley A., "Maintenance Costs of Complex Equipment," 20 pp., Dec 1978 (Published By The American Society of Naval Engineers, Naval Engineers Journal, Vol. 91, No. 6, Dec 1979) AD A071 473

PP 245
Simpson, William R., "The Accelerometer Methods of Obtaining Aircraft Performance from Flight Test Data (Dynamic Performance Testing)," 403 pp., Jun 1979, AD A075 226

PP 246
Brechling, Frank, "Layoffs and Unemployment Insurance," 35 pp., Feb 1979 (Presented at the NBER Conference on "Low Income Labor Markets," Chicago, Jun 1978)

PP 248
Thomas, James A., Jr., "The Transport Properties of Dilute Gases in Applied Fields," 183 pp., Mar 1979

PP 249
Glasser, Kenneth S., "A Secretary Problem with a Random Number of Choices," 23 pp., Mar 1979

PP 250
Mangel, Marc, "Modeling Fluctuations in Macroscopic Systems," 26 pp., Jun 1979

PP 251
Trost, Robert P., "The Estimation and Interpretation of Several Selectivity Models," 37 pp., Jun 1979, AD A075 941

PP 252
Nunn, Walter R., "Position Finding with Prior Knowledge of Covariance Parameters," 5 pp., Jun 1979 (Published in IEEE Transactions on Aerospace & Electronic Systems, Vol. AES-15, No. 3, March 1979

PP 253
Glasser, Kenneth S., "The d-Choice Secretary Problem," 32 pp., Jun 1979, AD A075 225

PP 254
Mangel, Marc and Quanbeck, David B., "Integration of a Bivariate Normal Over an Offset Circle," 14 pp., Jun 1979

PP 255 – Classified, AD B051 441L

PP 256
Maurer, Donald E., "Using Personnel Distribution Models," 27 pp., Feb 1980, AD A082 218

PP 257
Thaler, R., "Discounting and Fiscal Constraints: Why Discounting is Always Right," 10 pp., Aug 1979, AD A075 224

PP 258
Mangel, Marc S. and Thomas, James A., Jr. "Analytical Methods in Search Theory," 86 pp., Nov 1979, AD A077 832

PP 259
Glass, David V.; Hsu, Ih-Ching; Nunn, Walter R. and Perin, David A., "A Class of Commutative Markov Matrices," 17 pp., Nov 1979, AD A077 833

PP 260
Mangel, Marc S. and Cope, Davis K., "Detection Rate and Sweep Width in Visual Search," 14 pp., Nov 1979, AD A077 834

PP 261
Vila, Carlos L.; Zvijac, David J. and Ross, John, "Franck Condon Theory of Chemical Dynamics. VI Angular Distributions of Reaction Products," 14 pp., Nov 1979 (Reprinted from Journal Chem. Phys. 70(12), 15 Jun 1979), AD A076 287

PP 262
Petersen, Charles C., "Third World Military Elites in Soviet Perspective," 50 pp., Nov 1979, AD A077 835

PP 263
Robinson, Kathy I., "Using Commercial Tankers and Containerships for Navy Underway Replenishment," 25 pp., Nov 1979, AD A077 836

PP 264
Weinland, Robert G., "The U.S. Navy in the Pacific: Past, Present, and Glimpses of the Future," 31 pp., Nov 1979 (Delivered at the International Symposium on the Sea, sponsored by the International Institute for Strategic Studies, The Brookings Institution and the Yomiuri Shimbun, Tokyo, 16-20 Oct 1978) AD A066 837

PP 265
Weinland, Robert G., "War and Peace in the North: Some Political Implications of the Changing Military Situation in Northern Europe," 18 pp., Nov 1979 (Prepared for presentation to the "Conference of the Nordic Balance in Perspective: The Changing Military and Political Situation," Center for Strategic and International Studies, Georgetown University, Jun 15-16, 1978) AD A077 838

PP 266
Utgoff, Kathy Classen, and Brechling, Frank, "Taxes and Inflation," 25 pp., Nov 1979, AD A081 194

PP 267
Trost, Robert P., and Vogel, Robert C., "The Response of State Government Receipts to Economic Fluctuations and the Allocation of Counter-Cyclical Revenue Sharing Grants," 12 pp., Dec 1979 (Reprinted from the Review of Economics and Statistics, Vol LXI, No. 3, August 1979)

PP 268
Thomason, James S., "Seaport Dependence and Inter-State Cooperation: The Case of Sub-Saharan Africa," 141 pp., Jan 1980, AD A081 193

PP 269
Weiss, Kenneth G., "The Soviet Involvement in the Ogaden War," 42 pp., Jan 1980 (Presented at the Southern Conference on Slavic Studies in October, 1979), AD A082 219

PP 270
Remnek, Richard, "Soviet Policy in the Horn of Africa: The Decision to Intervene," 52 pp., Jan 1980 (To be published in "The Soviet Union in the Third World: Success or Failure," ed. by Robert H. Donaldson, Westview Press, Boulder, Co., Summer 1980), AD A081 195

PP 271
McConnell, James, "Soviet and American Strategic Doctrines: One More Time," 43 pp., Jan 1980, AD A081 192

PP 272
Weiss, Kenneth G., "The Azores in Diplomacy and Strategy, 1940-1945, 46 pp., Mar 1980, AD A085 094

PP 273
Nakada, Michael K., "Labor Supply of Wives with Husbands Employed Either Full Time or Part Time," 39 pp., Mar 1980, AD A082 220

PP 275
Goldberg, Lawrence, "Recruiters Advertising and Navy Enlistments," 34 pp., Mar 1980, AD A082 221

PP 276
Goldberg, Lawrence, "Delaying an Overhaul and Ship's Equipment," 40 pp., May 1980, AD A085 095

PP 277
Mangel, Marc, "Small Fluctuations in Systems with Multiple Limit Cycles," 19 pp., Mar 1980 (Published in SIAM J. Appl. Math., Vol. 38, No. 1, Feb 1980)

PP 278
Mizrahi, Maurice, "A Targeting Problem: Exact vs. Expected-Value Approaches," 23 pp., Apr 1980, AD A085 096

PP 279
Walt, Stephen M., "Causal Inferences and the Use of Force: A Critique of Force Without War," 50 pp., May 1980, AD A085 097

PP 280
Goldberg, Lawrence, "Estimation of the Effects of A Ship's Steaming on the Failure Rate of its Equipment: An Application of Econometric Analysis," 25 pp., April 1980, AD A085 098

PP 283
Dismukes, Bradford, "Expected Demand for the U.S. Navy to Serve as An Instrument of U.S. Foreign Policy: Thinking About Political and Military Environmental Factors," 30 pp., April 1980, AD A085 099

PP 284
J. Keilson,* W. Nunn, and U. Sumita,** "The Laguerre Transform," 119 pp., May 1980
*The Graduate School of Management, University of Rochester and the Center for Naval Analyses
**The Graduate School of Management, University of Rochester, AD A085 100

PP 285
Remnek, Richard B., "Superpower Security Interests in the Indian Ocean Area," 26 pp., Jun 1980

PP 287
Cope, Davis, "Limit Cycle Solutions of Reaction-Diffusion Equations," 325 pp., June 1980