NONLINEAR ANALYSIS

VOLUME I

N.M. TEMME (ed.)

MC SYLLABUS 26.1

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MATHEMATISCH CENTRUM AMSTERDAM 1976

AMS(MOS) subject classification scheme (1970): 00A10, 26A57, 34-01, 34CXX,
46-01, 47HXX.

ISBN 90 6196 117 3

CONTENTS

INTRODUCTION

In January 1975, the department of Applied Mathematics of the Mathematical Centre initiated a colloquium on Nonlinear Analysis under supervision of H.A. Lauwerier and L.A. Peletier. This book contains the first part of the proceedings of the lectures of this colloquium. It covers the lectures of the first quarter of 1975.

When choosing the topics from nonlinear analysis for the colloquium, the starting point was to give a mathematical introduction for workers in this field, especially those from applied mathematics, physics, biochemics and biology. For these workers no much accessible literature is available and this group needs, apart from the theory, clear examples of applying nonlinear analysis.

In chapters I, III and V we give such examples in such a way that each of these chapters can be understood without knowledge of the examples of the other chapters. Sometimes there is some interaction between them. The development of the theory is given in chapters II and IV.

Chapter I is of introductory nature. It treats a typical example from nonlinear analysis. In chapter II the analytic approach to the concept of topological degree of a continuous mapping $f\colon \mathbb{R}^n \to \mathbb{R}^n$ is given. Both the definition and the properties of degree are discussed extensively. The theory of this chapter is applied on several fixed point theorems. In chapter III some aspects of the theory of ordinary differential equations describing chemically reacting systems are considered. The main topics are the a priori bounds of solutions and the existence and stability of equilibrium points the latter aspects being considered by using degree theory developed in chapter II. In chapter IV nonlinear eigenvalue problems are discussed. The equation is $F(x,\lambda) = 0$, $x \in \mathbb{R}^n$, $\lambda \in \mathbb{R}$. A wide choice of illustrative examples is given, especially on bifurcation theory and on stability of solutions. In chapter V an example is given of branching of a set of periodic solutions from a constant solution of a predator-prey differential equation describing two interacting populations.

The results and examples in this book are not new. Apart from minor details all of the contents can be found in the literature.

Thanks to the effort of every member of our department the colloquium was very succesful. The lectures were prepared in working groups and were given by

L.A. Peletier (TH Delft)	chapter I
T.H. Koornwinder	chapter II
N.M. Temme	chapter III
O. Diekmann	chapter IV
I.G. Sprinkhuizen-Kuyper	chapter V.

The pictures were made by G.J.M. Laan.

The second volume in this series on Nonlinear Analysis will contain the proceedings of lectures on functional analysis, bifurcation theory for operators on a Banach space, the topological degree of mappings in Banach spaces, some nonlinear problems from physics, and variational methods for nonlinear operator equations.

December 1975 N.M. Temme

I. A NONLINEAR EIGENVALUE PROBLEM FROM CHEMICAL ENGINEERING

In this series of lectures the central theme will be the study of *nonlinear eigenvalue problems* and, in particular those which are found in physics, chemistry and biology. By a nonlinear eigenvalue problem we mean the problem of finding solutions of an equation of the form

(1) $\quad F(u,\lambda) = 0.$

Here F is some nonlinear operator and λ a real or complex valued parameter.

It is well known that the class of such problems for which the solutions can be found explicitly is very small. Thus for quantitative information one is very much dependent on numerical computations. However, in recent years powerful methods have been developed for obtaining information about the solutions which is qualitative in nature. They enable one to answer questions such as

(i) does (1) have a solution for a given value of λ;

(ii) if it does, how many solutions does it have;

(iii) how does this number vary with λ?

Such questions arise quite naturally in the interpretation of numerical results. This has been an important motivation for their study.

The methods used to answer these questions tend to rely on concepts and results taken from what is traditionally regarded as the realm of pure mathematics. Especially, elements of topology and functional analysis play a crucial role. In the course of this colloquium therefore, we shall also devote some time to these mathematical prerequisites. However, throughout the emphasis will be on the study of specific examples taken from various branches of science.

As an illustration of the questions we shall be interested in, we consider an example taken from chemical engineering. It involves the simultaneous occurrence of a catalytic reaction and mass transfer through diffusion.

We consider a infinite slab of homogeneous, chemically inert material. On the faces of this slab is situated a catalyst material. Outside the slab, the reactant is present with a constant and uniform concentration C_e. This situation is not entirely unrealistic. For instance it is an appropriate model for the exhaust filters that the US automotive industry has been trying out.

Let us choose the x-axis perpendicular to the slab, and position the origin of coordinates so that the two faces are at $x = 0$ and $x = \ell$. Then the concentration of the reactant $C(x,t)$ satisfies the differential equation

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad \text{for } 0 < \ell,\ t > 0,$$

together with the boundary conditions

$$C_e - C = -\frac{D}{K}\frac{\partial C}{\partial x} + r(C) \quad \text{for } x = 0,\ t > 0,$$

$$C_e - C = \frac{D}{K}\frac{\partial C}{\partial x} + r(C) \quad \text{for } x = \ell,\ t > 0.$$

Here the diffusion coefficient D and the coefficient of mass transfer at the surface K are positive constants. The function $r(C)$ represents the rate of consumption of the reactant. An appropriate choice for this function would be

$$r(C) = k_1 C\{1 + k_2\ (C/C_e)\}^{-2},$$

where k_1 and k_2 are positive constants. Finally, to complete the formulation of the problem we have to add the concentration profile at $t = 0$:

$$C(x,0) = C_0(x) \quad \text{for } 0 < x < \ell.$$

To simplify the statement of the problem we introduce dimensionless variables x/ℓ, Dt/ℓ^2, C/C_e for x,t and C respectively. In the new independent variables, which we again call x and t, $u = C/C_e$ satisfies the differential equation

$$u_t = u_{xx} \quad \text{for } 0 < x < 1,\ t > 0 \tag{2}$$

and the boundary conditions

(3) $$u_x(0,t) = +\lambda f(u(0,t) \quad \text{for } t > 0,$$

(4) $$u_x(1,t) = -\lambda f(u(1,t)) \quad \text{for } t > 0,$$

where $\lambda = K\ell/D$ is the Nusselt number and

$$f(u) = C_e^{-1} r(C_e u) + u - 1.$$

We shall assume that the constants k_1 and k_2 are such that the equation

$$f(u) = 0$$

has exactly three positive solutions u_i with $0 < u_1 < u_2 < u_3$. At $t = 0$ we choose

(5) $$u(x,0) = \Psi(x) \quad \text{for } 0 \le x \le 1.$$

Thus u must satisfy a linear equation and a pair of nonlinear boundary conditions. The initial-boundary value problem is therefore a nonlinear one.

To begin with, we would like to investigate the existence and multiplicity of equilibrium solutions of this problem for a given value of λ. Let $u(x)$ be such an equilibrium solution. Then it follows from the differential equation that $u''(x) = 0$, and hence, that we can write u as

$$u(x) = p + (\overset{q}{\cancel{1}}-p)\, x.$$

Clearly, $u(0) = p$ and $u(1) = q$. The boundary conditions are also satisfied if p and q satisfy the equations

$$q - p = +\lambda f(p),$$

$$q - p = -\lambda f(q).$$

We can write this as

(6) $$p = F_\lambda(u) = u + \lambda(q), \; q = F_\lambda(p),$$

where

$$F_\lambda(u) = u + \lambda f(u).$$

We observe that $(p,q) = (u_i,u_i)$, $i = 1,2,3$ are solutions of problem (6) for all values of λ. In fact these are the only symmetric solutions i.e. solutions for which $p = q$.

To investigate the existence of asymmetric solutions, we use the (p,q) plane. In this plane, solutions of (6) correspond to intersections of the graphs of $p = F_\lambda(q)$ and $q = F_\lambda(p)$. Since every asymmetric solution $(\bar{p},\bar{q})$ is accompanied by its dual $(\bar{q},\bar{p})$ it suffices to consider only the octant $q > p \geq 0$. If there exists a solution in this octant, it must occur in the set $S = \{(p,q) : u_1 < p < u_2, u_2 < q <\}$. However, it is clear that for λ sufficiently small, no points of the graph $\{F_\lambda(q),q): u_2 < q < u_3\}$ lie in this set. Hence, there exists a $\sigma^* \in (0,\infty)$ such that (6) has no asymmetric solutions for any value of $\lambda \in (0,\sigma^*)$.

Suppose (p,q) is an asymmetric solution of (6). Then p and q satisfy the relations

$$\text{(7)} \qquad \frac{f(q) - f(p)}{q-p} = -2/\lambda,$$

$$\text{(8)} \qquad f(p) = - f(q).$$

Conversely, if p and q satisfy (7) and (8), then (p,q) is a solution of (6).

We shall assume that

$$f(\alpha) = \max_{[u_1,u_3]} f(u) < \left| \min_{[u_1,u_3]} f(u) \right| = -f(\beta).$$

Then, since f is strictly decreasing on $[u_2,\beta)$, there exists a unique $\tilde{u} \in (u_2,\beta)$ such that $f > - f(\alpha)$ on $[u_2,\tilde{u})$ and $f(\tilde{u}) = f(\alpha)$.
Thus, to each $p \in [u_1,u_2]$ there corresponds a unique $q_1(p) \in [u_2,\tilde{u}]$ and a unique $\lambda_1(p)$ such that (7) and (8) are satisfied. Similarly, since f is strictly increasing on $(\beta,u_3]$ there exists a unique $\bar{u} \in [\beta,u_3]$ such that $f > -f(\alpha)$ on $(\bar{u},u_3]$ and $f(\bar{u}) = -f(\alpha)$. Hence, to each $p \in [u_1,u_2]$ there corresponds a unique $q_2(p) \in [\bar{u},u_3]$ and a unique $\lambda_2(p)$ such that (7) and (8) are satisfied.

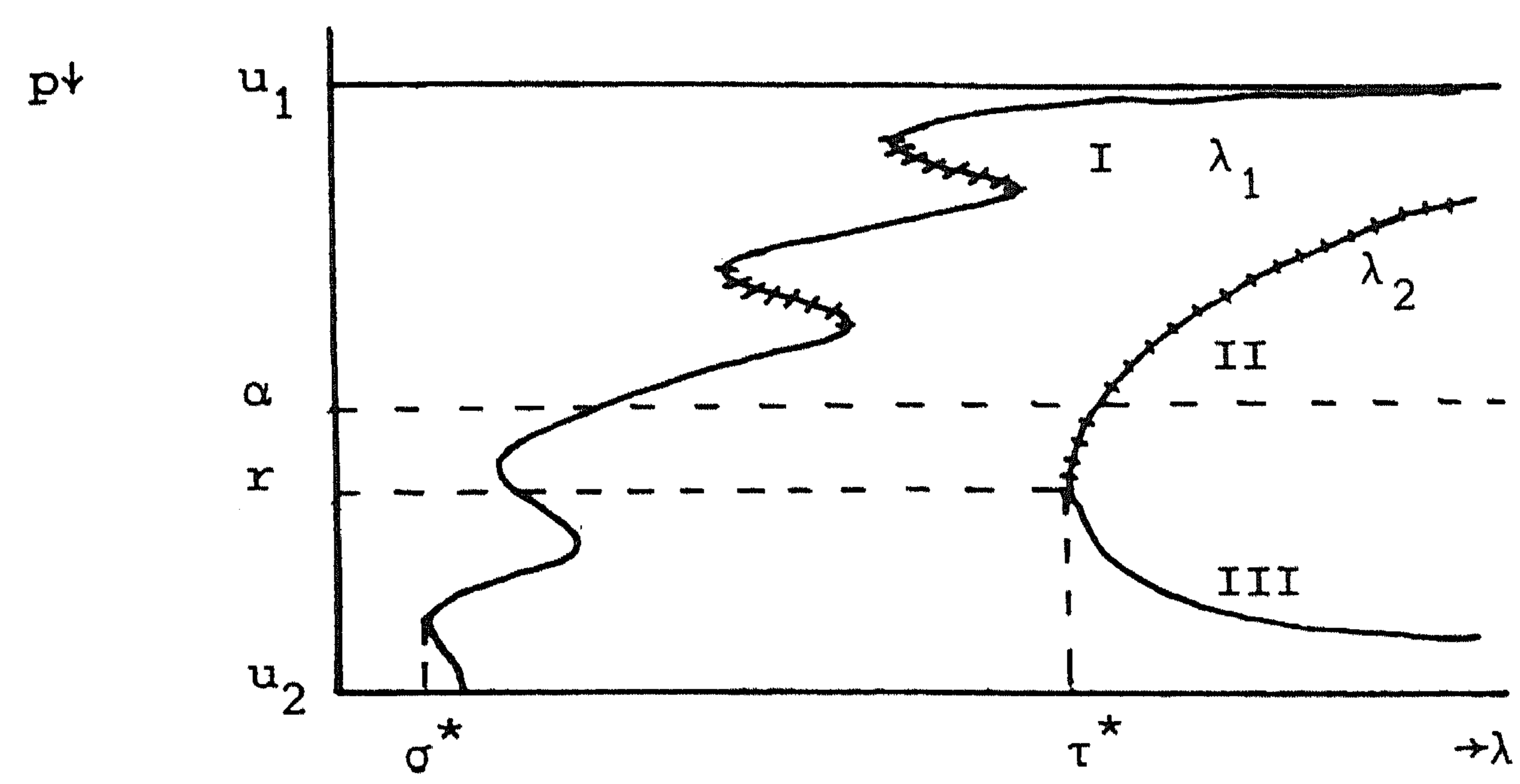

Figure 1

<u>REMARK 1</u>. If $p \downarrow u_1$, it follows from (8) that $q_1 \downarrow u_2$ and $q_2 \uparrow u_3$. Hence by (7) $\lambda_1 \to \infty$ and $\lambda_2 \to \infty$.

<u>REMARK 2</u>. If $p \uparrow u_2$, it follows from (8) that $q_1 \downarrow u_2$ and $q_2 \uparrow u_3$. Hence, by (7) $\lambda_1 \to -2/f'(u_2)$ and $\lambda_2 \to \infty$.

<u>REMARK 3</u>. In view of the construction $q_1(p) < q_2(p)$ for all $p \in [u_1,u_2]$. Hence, by (7) and (8), $\lambda_1(p) < \lambda_2(p)$ on $[u_1,u_2]$.

We observe that for $p = u_2$ and $\lambda = -2/f'(u_2)$ an equilibrium solution branches off the solution curve $\{(u_2,\lambda): \lambda \in \mathbb{R}\}$. This phenomenon is called *bifurcation*. It is one way in which new solutions can come into existence when λ varies. That it is not the only way is also shown by this example: at the point (r,τ^*) two solutions emerge which do not branch off another solution.

The solutions $(u_2,-2/f'(u_2))$ and (r,τ^*) have in common that their multiplicities are greater than 1. Solutions with this property can be found by means of the determinant of the system (6):

$$\lambda f'(p) + \lambda f'(q) + \lambda^2 f'(p)f'(q) = \lambda\delta(p,q,\ ).$$

For if $(\bar{p},\bar{q})$ is a solution of (6), then $(\bar{p},\bar{q})$ has multiplicity ≥ 2 if and only if $\delta(\bar{p},\bar{q},\lambda) = 0$. To show this we observe that solutions of (6) are in one to one correspondence with the roots of the equation

$$F(q) \equiv f(q) + f(F_\lambda(q)) = 0.$$

Because

$$F'(q) = f'(q) + f'(F_\lambda(q))\{1 + f'(q)\} = \delta(p,q,\lambda)$$

the result follows at once.

For applications it is often important to know whether any of the equilibrium solutions constructed above are stable. That is, one would like to know the relationship between the equilibrium solutions and the solutions $u(x,t;\Psi)$ of the initial-boundary value problem (2)-(5). In particular, given an equilibrium solution $\bar{u}(x) = \bar{p} + (\bar{q}-\bar{p})x$, one would like to know for which functions Ψ, $u(x,t;\Psi) \to \bar{u}(x)$ as $t \to \infty$ uniformly in x. It is possible to show that if Ψ is close enough to an equilibrium solution $\bar{u}$, for which $(\lambda(\bar{p}),\bar{p})$ belongs to the cross hatched arcs in the (p,λ) plane, then $u(.,t;\Psi) \to \bar{u}$ as $t \to \infty$. Such equilibrium solutions are called asymptotically stable. The equilibrium solutions corresponding to the remaining parts of the graphs in the (p,λ) plane are all unstable. The methods, by which these results are obtained, rely on the maximum principle.

LITERATURE

[1] ARONSON, D.G. & L.A. PELETIER, *Global stability of symmetric and asymmetric concentration profiles in catalyst particles*, Arch. Rat. Mech. Anal. 54 (1974) 175-204.

II. THE TOPOLOGICAL DEGREE OF A MAPPING

In this chapter we shall give an analytic approach to the concept of degree of a mapping. For an approach using combinatorial topology, which is closer to Brouwer's original theory, we refer to CRONIN [1]. In order to understand applications in subsequent chapters it is sufficient to read subsections 2.1, 2.2, 2.3, section 3 and subsection 4.1.

1. MOTIVATION

Throughout this chapter Ω will be an open bounded subset of the n-dimensional real vector space $\mathbb{R}^n$. The closure of Ω wil be denoted by $\bar{\Omega}$ and $\partial\Omega$ will be the boundary of Ω. As a concrete example the reader may take for Ω the open unit ball in $\mathbb{R}^n$. Then $\partial\Omega$ is the unit sphere S^{n-1}.

Let $f\colon \Omega \to \mathbb{R}^n$ be a continuous mapping and let $p \in \mathbb{R}^n$ be such that $f(x) \neq p$ for each $x \in \partial\Omega$, i.e. $p \in \mathbb{R}^n - f(\partial\Omega)$. It is our aim to get information about the solutions in Ω of the equation

$$f(x) = p. \tag{1.1}$$

In general, this is a nonlinear equation which cannot be solved in an explicit way. However, we shall obtain qualitative information about the solutions of (1.1) by associating with each triple (f,Ω,p) an integer

$$\deg(f,\Omega,p)$$

such that the following properties hold.

<u>PROPERTY 1.1</u>. (*Homotopy invariance*)
Let the mapping $(x,t) \to f_t(x)$ be continuous from $\bar{\Omega} \times [0,1]$ into $\mathbb{R}^n$ and let

$f_t(x) \neq p$ if $(x,t) \in \partial\Omega \times [0,1]$. Then $\deg(f_t,\Omega,p)$ is independent of t.

PROPERTY 1.2. (*Boundary value dependence*)
If Ω and p are fixed then $\deg(f,\Omega,p)$ is uniquely determined by the restriction of f to the boundary $\partial\Omega$.

We shall call $\deg(f,\Omega,p)$ the (topological) *degree* of the mapping f with respect to the region Ω and the point p. It will be helpful for the reader to think about two distinct spaces $\mathbb{R}^n$, say X and Y, such that X includes the domain $\bar{\Omega}$ of f and Y contains the point p and the range $f(\bar{\Omega})$ of f.

In our approach a particular class of nice mappings, say a class F, will be selected such that an arbitrary continuous mapping can be continuously deformed to an element of F. For $f \in F$ a simple analytic definition of degree will be given. If this definition can be extended to the case of general f then we know the degree of an arbitrary f by homotopy invariance (cf. property 1.1). Such an extension will indeed be possible.

It will be proved that equation (1.1) has at least one solution $x \in \Omega$ if $\deg(f,\Omega,p) \neq 0$. This theorem may give the reader an idea about the usefulness of the concept of degree.

Suppose that f maps $\bar{\Omega}$ into $\bar{\Omega}$. Then the equation

$$f(x) = x, \tag{1.2}$$

which can be considered as a special case of (1.1), is of particular importance. If for each continuous mapping $f: \bar{\Omega} \to \bar{\Omega}$ equation (1.2) has at least one solution in $\bar{\Omega}$ then $\bar{\Omega}$ is said to have the *fixed point property*. We shall prove the fixed point property for the closed ball (Brouwer's theorem) by using the concept of degree.

In order to get some feeling about the subject we shall first discuss the one- and two-dimensional cases.

1.1. THE ONE-DIMENSIONAL CASE

Let Ω be the open interval $(-1,1)$. Then $\bar{\Omega}$ is the closed interval $[-1,1]$ and $\partial\Omega$ consists of the points -1 and 1. First we prove Brouwer's fixed point theorem for $\bar{\Omega} = [-1,1]$.

THEOREM 1.3. *Let the function* $f: [-1,1] \to [-1,1]$ *be continuous. Then equation* (1.2) *has at least one solution in* $[-1,1]$.

<u>PROOF</u>. (Cf. figure 1). Suppose that (1.2) has no solutions for $x = \pm 1$. Let $g(x) = x - f(x)$. Then $g(-1) < 0$ and $g(1) > 0$. By the intermediate value theorem $g(x) = 0$ somewhere on $(-1,1)$. □

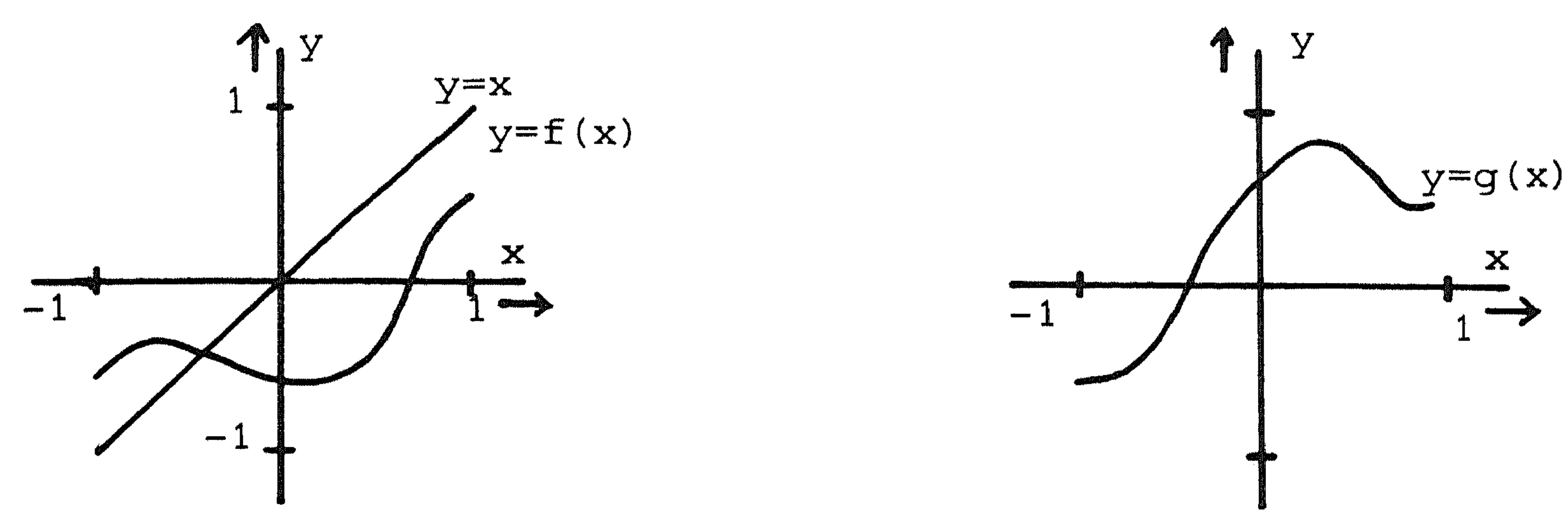

Figure 1

Next, let the function $f: [-1,1] \to \mathbb{R}$ be continuous and let $p \in \mathbb{R}$ such that $f(x) \neq p$ for $x = \pm 1$. A first candidate for $\deg(f,(-1,1),p)$ might be the number of solutions of equation (1.1) in the interval $(-1,1)$. However, this number does not have the property of homotopy invariance. For instance, the equation $x^2 + t = 0$ has zero, one or two solutions on $(-1,1)$ according to whether $t > 0$, $t = 0$ or $-1 < t < 0$ (cf. figure 2).

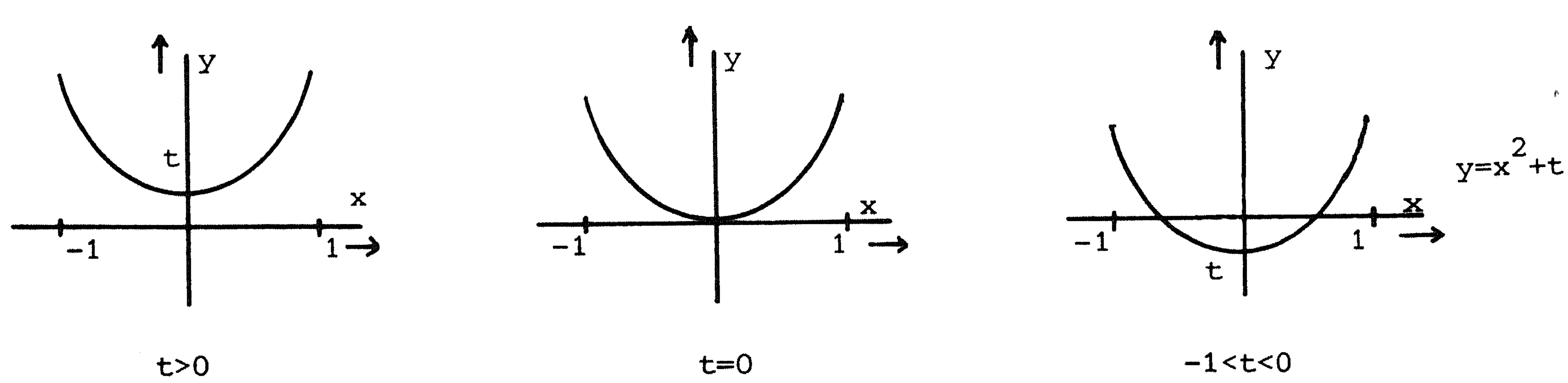

Figure 2

Let us try another definition of degree. Let F be a class of "nice" functions consisting of all continuous functions $f: [-1,1] \to \mathbb{R}$ such that $f(\pm 1) \neq p$ and the set $f^{-1}(p)$ of solutions of (1.1) is finite. Note that

$f^{-1}(p)$ may be empty for $f \in \mathcal{F}$. Let $f^{-1}(p)$ consist of k distinct points $x_1,\ldots,x_k \in (-1,1)$. With each x_i, $i = 1,\ldots,k$, we associate a number σ_i which is equal to 1,-1 or 0 according to whether f is increasing, decreasing or has local extremum in x_i. Then we define

$$\deg(f,(-1,1),p) = \sum_{i=1}^{k} \sigma_i . \tag{1.3}$$

In the example of figure 3, $\sigma_1 = -1$, $\sigma_2 = 0$, $\sigma_3 = 1$ and the degree of f is zero.

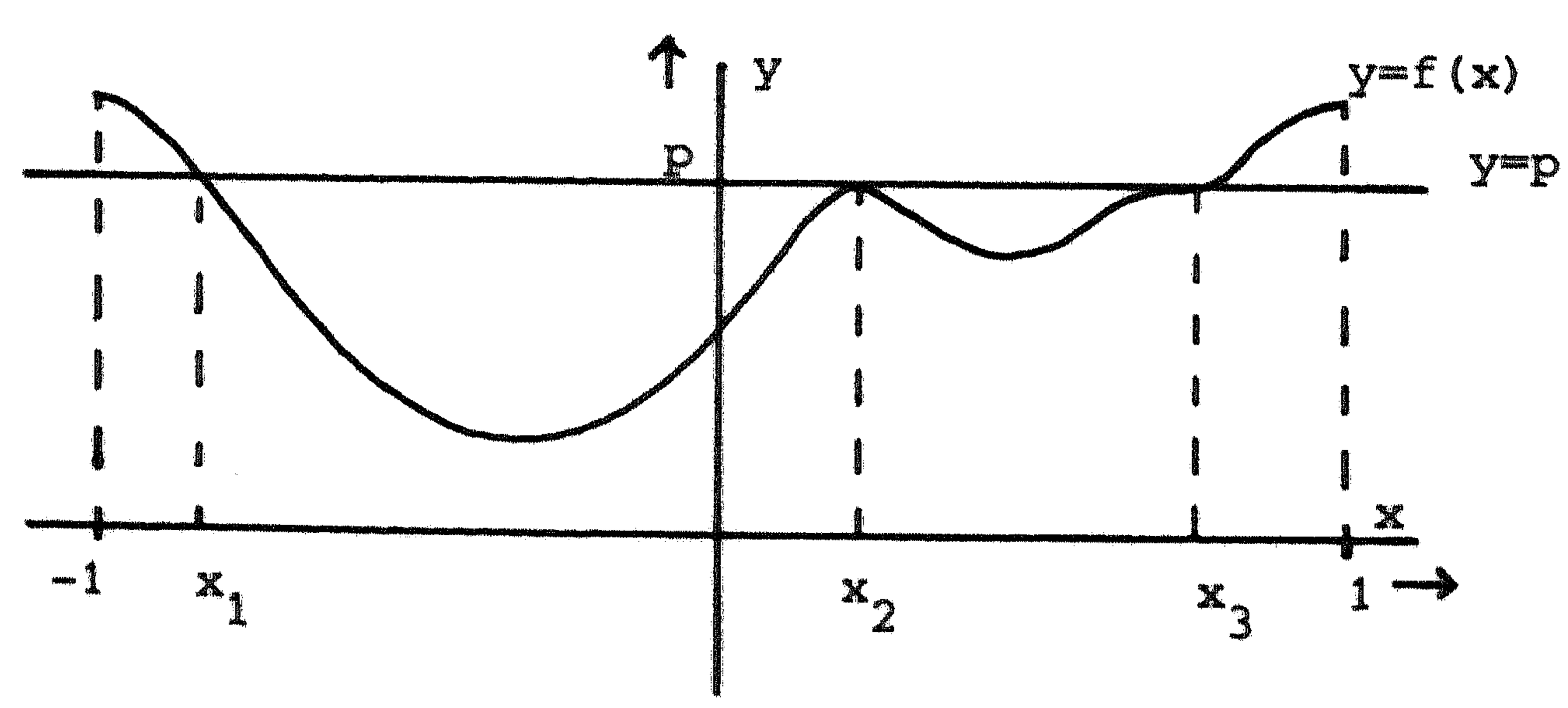

Figure 3

The following result is easily verified.

<u>LEMMA 1.4</u>. *Let the degree of* $f \in \mathcal{F}$ *be defined by* (1.3). *Then* $\deg = 1$ *if* $f(-1) - p < 0$, $f(1) - p > 0$; $\deg = -1$ *if* $f(-1) - p > 0$, $f(1) - p < 0$; $\deg = 0$ *if* $f(-1) - p$ *and* $f(1) - p$ *have equal signs. In other words*

$$\deg(f,(-1,1),p) = \tfrac{1}{2}\left[\frac{f(1) - p}{|f(1) - p|} - \frac{f(-1) - p}{|f(-1) - p|}\right] . \tag{1.4}$$

Formula (1.4) gives an extension of definition (1.3) for general continuous $f\colon [-1,1] \to \mathbb{R}$ such that $f(1) \neq p$. This definition of degree satisfies the properties 1.1 and 1.2. In fact, formula (1.4) is the only possible extension of the case $f \in \mathcal{F}$ if property 1.1 is assumed. For proving this let

$$f_t(x) = t[\tfrac{1}{2}(1+x)f(1) + \tfrac{1}{2}(1-x)f(-1)] + (1-t)f(x), \tag{1.5}$$

then $f_t(x)$ is of the form required in property 1.1. Note that

$$f_0 = f, \qquad f_1(x) = \tfrac{1}{2}(1+x)f(1) + \tfrac{1}{2}(1-x)f(-1), \qquad f_t(\pm 1) = f(\pm 1).$$

Then $f_1 \in F$ and f and f_1 must have the same degree by property 1.1.

The boundary values $f(-1)$ and $f(1)$ divide the real line into two or three intervals (connected components). On each of these components the degree is a constant function of p. However, if p passes a boundary value then the degree may change. Hence, there is no satisfactory way to define the degree if p is a boundary value of f. Note that the degree is always zero on the two unbounded components of $\mathbb{R} - \{f(-1), f(1)\}$. Figure 4 gives one possible siatuation.

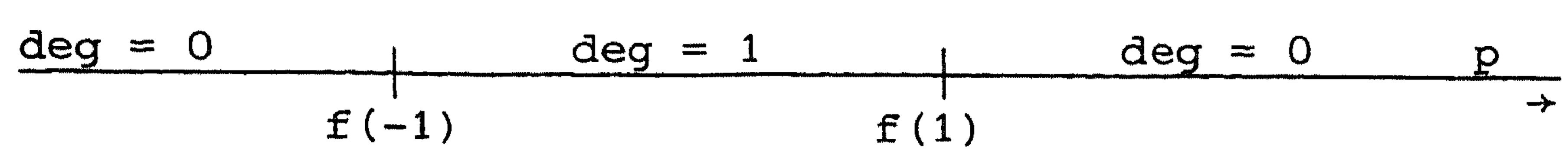

Figure 4

Finally, in view of generalization to higher dimension, consider continuous functions $f\colon [-1,1] \to \mathbb{R}$, which are continuously differentiable on $(-1,1)$. If $f(\pm 1) \neq p$ and if $f'(x) \neq 0$ for $x \in f^{-1}(p)$ then $f^{-1}(p)$ is a finite set and (1.3) is equivalent with

$$\deg(f,(-1,1),p) = \sum_{x \in f^{-1}(p)} \operatorname{sign} f'(x). \tag{1.6}$$

1.2. ANALYTIC FUNCTIONS ON THE DISK

Let Ω denote the open unit disk $\{z \in \mathbb{C} \mid |z| < 1\}$ in the complex plane $\mathbb{C}$. Suppose that f is a nonconstant analytic function on the closed unit disk $\bar{\Omega}$ and let $p \in \mathbb{C}$ such that $p \in \mathbb{C} - f(\partial\Omega)$. Then $f^{-1}(p) = \{z_1, \ldots, z_k\}$ is a finite (possibly empty) subset of Ω. Let σ_j be the multiplicity of the zero z_j of $f - p$, i.e., $f(z) - p = c(z-z_j)^{\sigma_j} + O(|z - z_j|^{\sigma_j+1})$, $c \neq 0$. We define the degree of f by

$$\deg(f,\Omega,p) = \sum_{j=1}^{k} \sigma_j, \tag{1.7}$$

i.e. the number of zeros of $f - p$ in Ω counted by their multiplicities. In §1.1 we remarked that for a similar definition in the one-dimensional case property 1.1 does not hold, cf. figure 2. However, in the present case property 1.1 is satisfied as long as we restrict ourselves to analytic functions f. In fact, Rouche's theorem (cf. TITCHMARSH [2, §3.42]) implies that if g is analytic on $\bar{\Omega}$ and if $\max_{z\in\partial\Omega}|g(z)| < \min_{z\in\partial\Omega}|f(z) - p|$ then $\deg(f,\Omega,p) = \deg(f+g,\Omega,p)$. This settles property 1.1 for functions $f_t(z)$ which are analytic in z for each $t \in [0,1]$.

Let the degree be defined by (1.7). Using elementary complex analysis we rewrite (1.7) as

$$\deg(f,\Omega,p) = \frac{1}{2\pi i}\oint_{\partial\Omega} \frac{f'(z)}{f(z) - p}\,dz = \frac{1}{2\pi i}\oint_{\partial\Omega} d\log(f(z)-p) = \tag{1.8}$$

$$= \frac{1}{2\pi}\oint_{\partial\Omega} d\arg(f(z)-p).$$

Hence the degree only depends on the restriction of f to the boundary. Therefore property 1.2 is satisfied.

Formula (1.8) gives a geometric interpretation of degree. It is the number of times that the image $f(\partial\Omega)$ encircles p. For instance, consider the example $f(z) = 2z^2 + z$. In figure 5 it is shown how the degree depends on p.

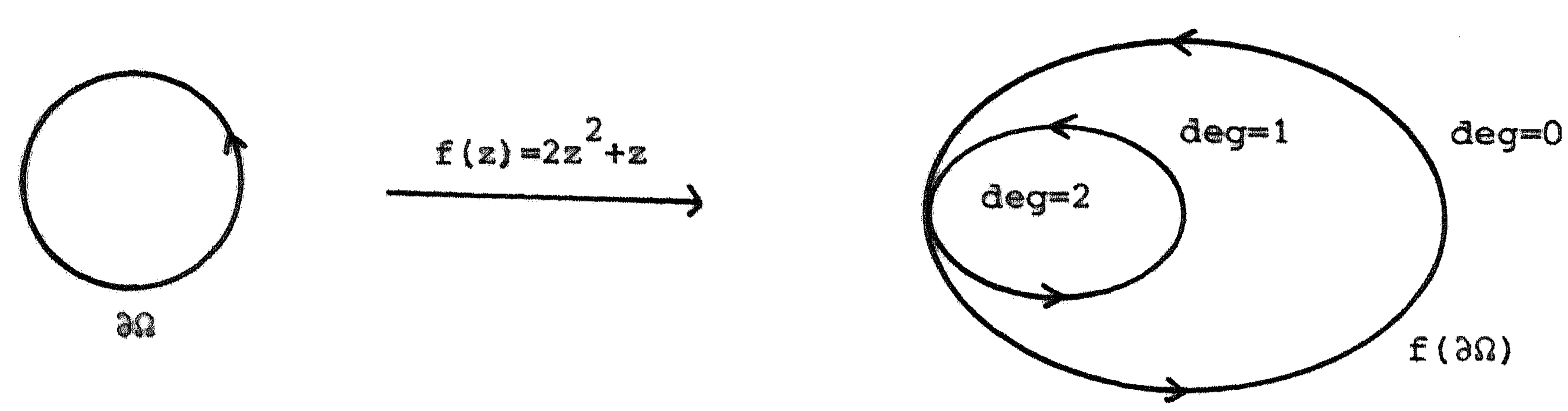

Figure 5

1.3. DEGREE THEORY IN $\mathbb{R}^2$

The last member of (1.8) is a good starting point for extending the definition of degree to the case that f is not analytic. Let Ω be the open unit disk $\{x = (x^1,x^2) \in \mathbb{R}^2 \mid (x^1)^2 + (x^2)^2 < 1\}$ in $\mathbb{R}^2$, let $f = (f^1,f^2)$ be a continuous mapping from $\bar{\Omega}$ into $\mathbb{R}^2$ and let $p = (p^1,p^2) \in \mathbb{R}^2 - f(\partial\Omega)$. Let the unit circle $\partial\Omega$ be parametrized by $x(\phi) = (\cos\phi,\sin\phi)$, $0 \le \phi \le 2\pi$. It is possible to define the angle $\arg(f(x(\phi))-p)$ as a continuous function of ϕ on the interval $[0,2\pi]$ such that

$$\operatorname{tg}\ \arg(f(x(\phi))-p) = \frac{f^2(x(\phi)) - p^2}{f^1(x(\phi)) - p^1}\ .$$

We then define the degree as the so-called *rotation* of $f - p$, i.e.,

$$\deg(f,\Omega,p) = (2\pi)^{-1}(\arg(f(x(2\pi))-p) - \arg(f(x(0))-p)). \tag{1.9}$$

If f is analytic then (1.9) is equivalent with (1.8). Geometrically, the degree as defined by (1.9) denotes the number of times that the image $f(\partial\Omega)$ encircles p, where an anticlockwise rotation is counted positively and a clockwise rotation negatively. An example is given in figure 6. Again, properties 1.1 and 1.2 easily follow from (1.9).

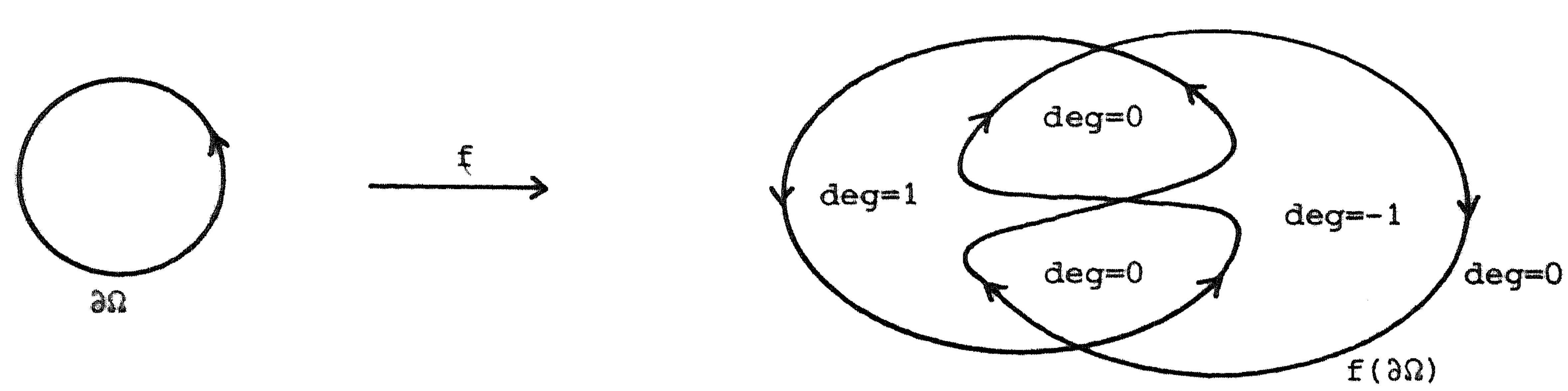

Figure 6

<u>THEOREM 1.5</u>. (*Brouwer's theorem for* $\mathbb{R}^2$)
Let Ω *be the open unit disk in* $\mathbb{R}^2$ *and let the mapping* $f\colon \bar{\Omega} \to \bar{\Omega}$ *be continuous. Then the equation* $f(x) = x$ *has at least one solution in* $\bar{\Omega}$.

<u>PROOF</u>. Suppose that f has no fixed points in $\bar{\Omega}$. Let $g(x) = x - f(x)$. Then g has no zeros in Ω. Define for $0 \le t \le 1$

$$g_t(x) = x - (1-t)f(x).$$

$$h_t(x) = \begin{cases} g((1-t)|x|^{-1}x) & \text{if } 1 - t < |x| \le 1, \\ g(x) & \text{if } |x| \le 1 - t. \end{cases}$$

Then both $g_t(x)$ and $h_t(x)$ are continuous in $(x,t) \in \bar{\Omega} \times [0,1]$ and $g_t(x) \ne 0 \ne h_t(x)$ if $x \in \partial\Omega$. Note that $g_0 = g = h_0$, $g_1(x) = x$, $h_1(x) = g(0)$. The degrees of g_1 and h_1 for $p = 0$ follow from (1.9). Property 1.1 gives

$1 = \deg(g_1,\Omega,0) = \deg(g,\Omega,0) = \deg(h_1,\Omega,0) = 0$. This is a contradiction. $\square$

If $f\colon \Omega \to \mathbb{R}^2$ is continuously differentiable on the closed unit disk Ω, then (1.9) can be rewritten as an integral over $\partial\Omega$. We have

$$(1.10)\qquad \deg(f,\Omega,p) = \frac{1}{2\pi}\oint_{\partial\Omega} d\ \mathrm{arctg}\left(\frac{f^2-p^2}{f^1-p^1}\right) = \\ = \frac{1}{2\pi}\oint_{\partial\Omega} \frac{(f^1-p^1)df^2 - (f^2-p^2df^1}{|f-p|^2}\ .$$

Let us finally try to extend (1.7) to the case that f is not analytic. Denote the determinant of the Jacobian of a differentiable mapping $(x^1,x^2) \to (f^1,f^2)$ by $J_f(x)$. Suppose that $f(z)$ is analytic and write $f(z) = f(x^1+ix^2) = f^1(x^1,x^2) + if^2(x^1,x^2)$. Then by the Cauchy-Riemann equations $J_f(x) = |f'(x^1+ix^2)|^2$. Hence, if $z = x^1 + ix^2$ is a simple root of $f(z) - p$ then $J_f(x) > 0$ for $x = (x^1,x^2)$.

Suppose now that $f\colon \bar\Omega \to \mathbb{R}^2$ is continuous on $\bar\Omega$ and continuously differentiable on Ω, let $p \in \mathbb{R}^2 - f(\partial\Omega)$ and let $f^{-1}(p)$ be a (possibly empty) finite set on which $J_f(x)$ is non-zero. Then we define

$$(1.11)\qquad \deg(f,\Omega,p) = \sum_{x\in f^{-1}(p)} \mathrm{sign}\ J_f(x)\ .$$

Formula (1.11) reduces to (1.7) if f is analytic and $f - p$ has simple roots. However, if f is not analytic then $J_f(x)$ may also have negative sign. Formula (1.11) is the two-dimensional analogue of (1.6). It can be proved that (1.11) is consistent with (1.9) and (1.10).

2. DEFINITION OF THE DEGREE $\deg(f,\Omega,p)$ IN $\mathbb{R}^n$

The definition of degree by analytic methods goes back to NAGUMO [3] and HEINZ [4]. Recent presentations of this theory are given by SCHWARTZ [5, chap. 3], BERGER & BERGER [6, chap. 2], FUČIK, NEČAS, SOUČEK & SOUČEK [7, chap. 1], NIRENBERG [8, chap. 1] and DEIMLING [9, chap. 2]. NIRENBERG [8] and SCHWARTZ [5] will be our main references in this section.

Let Ω be an open bounded subset of $\mathbb{R}^n$. Let $f\colon \bar{\Omega} \to \mathbb{R}^n$ be a continuous mapping, i.e. $f \in C(\bar{\Omega})$. Let $p \in \mathbb{R}^n - f(\partial\Omega)$. We shall define the degree $\deg(f,\Omega,p)$ in three stages. Some rather technical proofs will be postponed to an appendix at the end of this section.

2.1. FIRST STAGE: CONTINUOUSLY DIFFERENTIABLE FUNCTIONS f AND REGULAR VALUES p

Suppose that $f \in C(\bar{\Omega})$ and that for $x \in \Omega$ all partial derivatives $\frac{\partial f^i(x)}{\partial x^j}$ exist and are continuous. Then we shall write $f \in C(\bar{\Omega}) \cap C^1(\Omega)$. For $x \in \Omega$ let $J_f(x)$ denote the determinant of the Jacobian matrix

$$\begin{pmatrix} \frac{\partial f^1(x)}{\partial x^1} & \cdots & \frac{\partial f^1(x)}{\partial x^n} \\ \vdots & & \vdots \\ \frac{\partial f^n(x)}{\partial x^1} & \cdots & \frac{\partial f^n(x)}{\partial x^n} \end{pmatrix}$$

We introduce the following sets associated with the mapping f.

DEFINITION 2.1.

(a) $Z = \{x \in \Omega \mid J_f(x) = 0\}$ is the set of *critical points* of f.

(b) $\Omega - Z$ is the set of *regular points* of f.

(c) $f(Z)$ is the set of *critical values* of f.

(d) $\mathbb{R}^n - f(Z)$ is the set of *regular values* of f.

LEMMA 2.2. (*Implicit function theorem, special case*)
Let $x \in \Omega$ be a regular point of f. Then there is a neighborhood $U \subset \Omega$ of x such that f is a homeomorphic mapping from U onto $f(U)$ and the mapping $f^{-1}\colon f(U) \to U$ is continuously differentiable.

<u>LEMMA 2.3</u>. *Let* $p \in \mathbb{R}^n - f(\partial\Omega) - f(Z)$. *Then* $f^{-1}(p)$ *is a finite (possibly empty) subset of* Ω.

<u>PROOF</u>. The set $f^{-1}(p)$ is a closed subset of the compact set $\bar{\Omega}$. Hence $f^{-1}(p)$ is compact. Since $f^{-1}(p)$ consists of regular points of f it is by lemma 2.2 a discrete subset of Ω. Any compact discrete set is finite. $\square$

After these preparations we can give the first stage of the definition of degree.

<u>DEFINITION 2.4</u>. Let $f \in C(\bar{\Omega}) \cap C^1(\Omega)$ and $p \in \mathbb{R}^n - f(\partial\Omega) - f(Z)$. Then

$$\deg(f,\Omega,p) = \sum_{x \in f^{-1}(p)} \operatorname{sign} J_f(x). \tag{2.1}$$

This definition is the n-dimensional analogue of (1.6) and (1.11). Note that $\deg(f,\Omega,p)$ is *integer-valued*. Consider as an example the mapping f in figure 7.

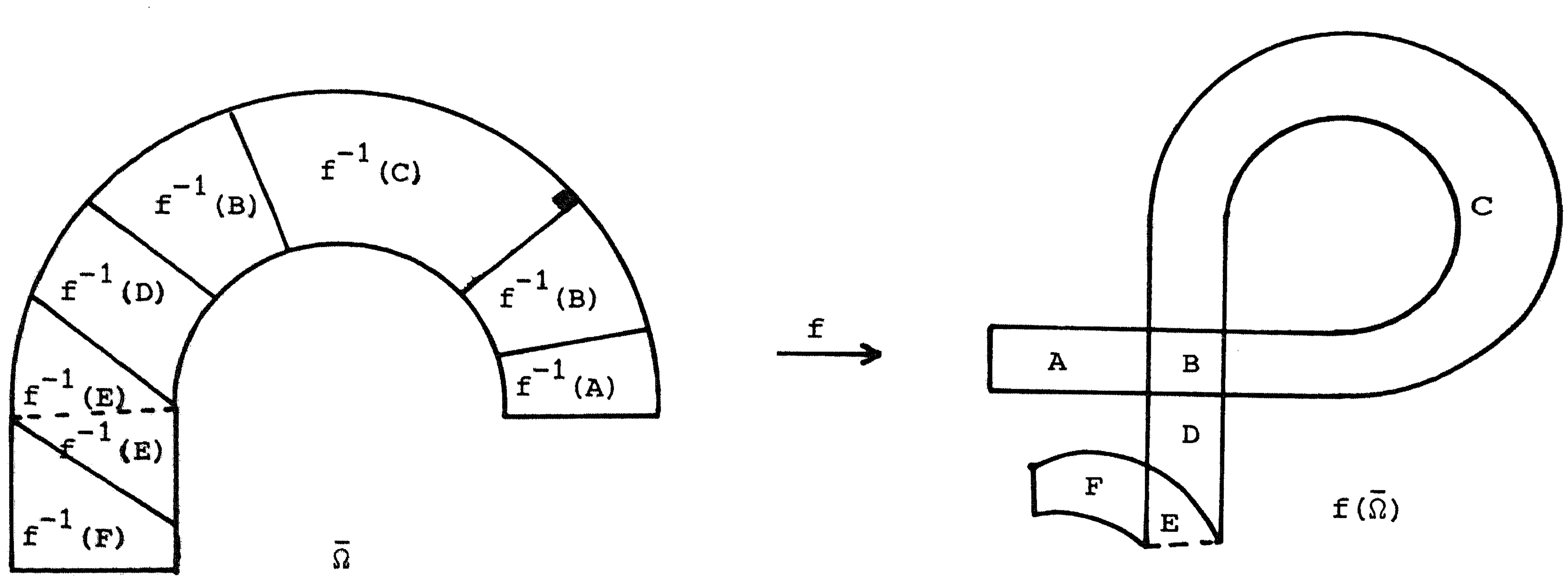

Figure 7

Then for the degree of f we have

p in	A	B	C	D	E	F	$\mathbb{R}^2 - f(\Omega)$
$\deg(f,p,\Omega) =$	1	2	1	1	0	−1	0

Table 1

In subsection 2.2 and 2.3 we shall extend definition 2.4 to the case that $f \in C(\bar{\Omega})$ and $p \in \mathbb{R}^n - f(\partial\Omega)$, such that $\deg(f,\Omega,p)$ is continuous in f and p (continuity in f with respect to the uniform topology for $C(\bar{\Omega})$). The possibility of such an extension has to be proved. However, the two following lemmas show that there exists at most one such extension.

<u>LEMMA 2.5</u>. (SARD)
Let $f \in C(\bar{\Omega}) \cap C^1(\Omega)$. *Then the subset* $f(Z)$ *of* $\mathbb{R}^n$ *has Lebesgue measure zero.*

This lemma will be proved in §2.4. It follows that $f(Z)$ cannot have interior points. The set $\mathbb{R}^n - f(\partial\Omega)$ is open. Hence, if $p \in f(Z)$ and $p \notin f(\partial\Omega)$ then each neighborhood of p has nonempty intersection with $\mathbb{R}^n - f(\partial\Omega) - f(Z)$.

<u>LEMMA 2.6</u>. *Let* $f \in C(\bar{\Omega})$. *For each* $\varepsilon > 0$ *there is a mapping* $g \in C(\bar{\Omega}) \cap C^1(\Omega)$ *such that* $\max_{x \in \bar{\Omega}} |f(x) - g(x)| < \varepsilon$.

It will be useful to rewrite the right-hand side of (2.1) as an integral.

<u>LEMMA 2.7</u>. *Let* $f \in C(\bar{\Omega}) \cap C^1(\Omega)$ *and* $p \in \mathbb{R}^n - f(\partial\Omega) - f(Z)$. *Let* $\deg(f,\Omega,p)$ *be defined by* (2.1). *Then there exists a positive number* r *such that for each continuous function* $\psi\colon \mathbb{R}^n \to \mathbb{R}$ *which vanishes on* $\{y \in \mathbb{R}^n \mid |y - p| > r\}$ *and which satisfies* $\int_{\mathbb{R}^n} \psi(y)dy = 1$ *the following holds:*

$$(2.2) \qquad \deg(f,\Omega,p) = \int_{\Omega} \psi(f(x)) J_f(x)dx.$$

<u>PROOF</u>. First suppose that $p \notin f(\bar{\Omega})$. Then $f^{-1}(p)$ is empty and $\deg(f,\Omega,p) = 0$ by (2.1). Since $\bar{\Omega}$ is compact, $f(\bar{\Omega})$ is compact and $\mathbb{R}^n - f(\bar{\Omega})$ is open. Choose $r > 0$ such that $|y - p| > r$ for each $y \in f(\bar{\Omega})$. If $\psi(y) = 0$ for $|y - p| > r$ then $\psi(f(x)) = 0$ for $x \in \Omega$. Hence the right-hand side of (2.2) also vanishes.

Next suppose that $p \in f(\bar{\Omega})$. Let $f^{-1}(p)$ consist of the points $x_1, x_2, \ldots, x_k$ $(k>0)$. By lemma 2.2 there are disjoint neighborhoods $U_1, U_2, \ldots, U_k$ of $x_1, x_2, \ldots, x_k$, respectively, such that $U_i \subset \Omega$, $J_f(x)$ has constant sign on each U_i, and the mappings $U_i \overset{f}{\to} f(U_i)$ and $f(U_i) \overset{f^{-1}}{\to} U_i$ are one-to-one and continuously differentiable. Let $U_0 = \bar{\Omega} - U_1 - U_2 - \ldots - U_k$. Then U_0 and $f(U_0)$ are compact and $p \notin f(U_0)$. Now we can choose $r > 0$ such that the set $W = \{y \in \mathbb{R}^n \mid |y - p| < 2r\}$ is included in $(\mathbb{R}^n - f(U_0)) \cap f(U_1) \cap f(U_2) \cap \ldots \cap f(U_k)$. Let $V_i = f^{-1}(W) \cap U_i$, $i = 1, \ldots, k$. Then $f^{-1}(W)$ is the disjoint union of the open sets $V_1,\dots,V_k$ and $x_i \in V_i$, cf. figure 8. Let $\psi\colon \mathbb{R}^n \to \mathbb{R}$ be continuous such that $\psi(y) = 0$ if $|y - p| > r$ and let $\int_{\mathbb{R}^n} \psi(y)\,dy = 1$. Then

$$\int_\Omega \psi(f(x))J_f(x)dx = \int_{f^{-1}(W)} \psi(f(x))J_f(x)dx = \sum_{i=1}^{k} \int_{V_i} \psi(f(x))J_f(x)dx =$$

$$= \sum_{i=1}^{k} (\operatorname{sign} J_f(x_i)) \int_{V_i} \psi(f(x))\ |J_f(x)|\ dx =$$

$$= \left(\sum_{i=1}^{k} \operatorname{sign} J_f(x_i)\right) \int_W \psi(y)dy =$$

$$= \deg(f,\Omega,p) \int_{\mathbb{R}^n} \psi(y)dy = \deg(f,\Omega,p). \qquad \square$$

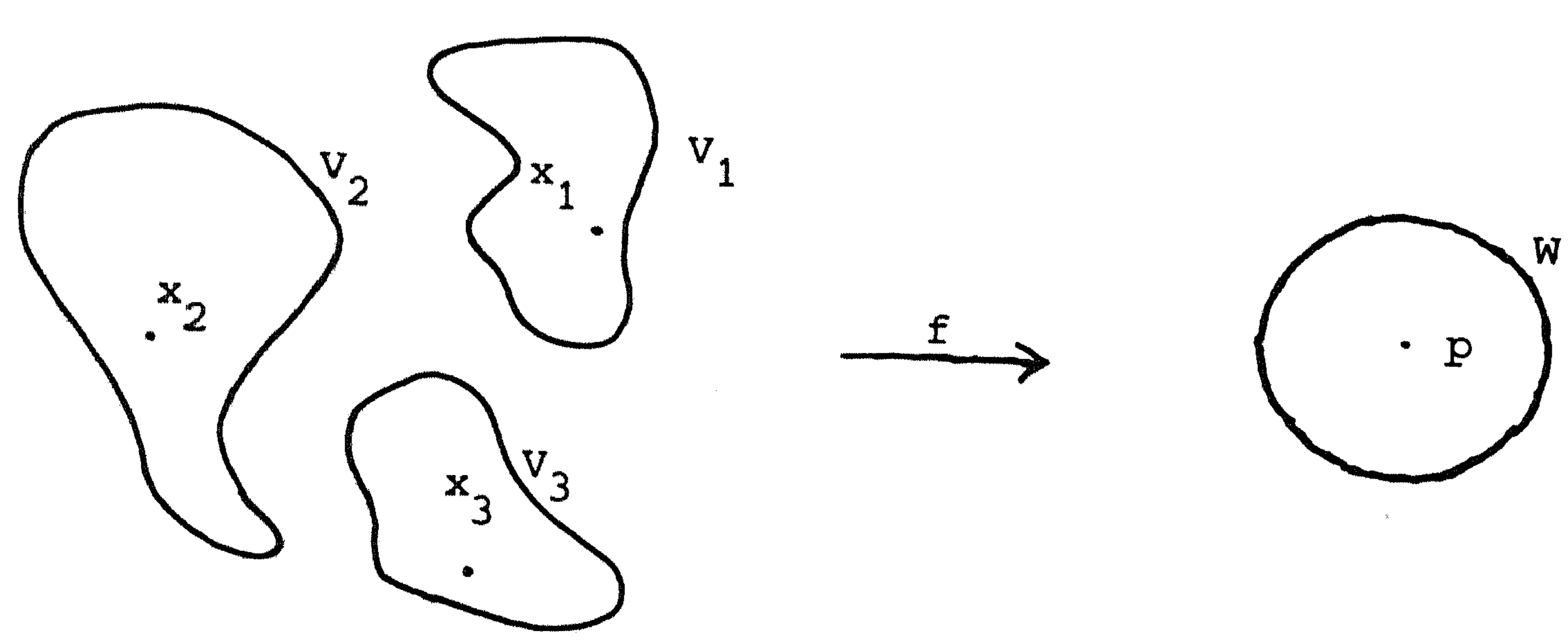

Figure 8

2.2. SECOND STATE: EXTENSION TO CRITICAL VALUES p

Suppose again that $f \in C(\bar{\Omega}) \cap C^1(\Omega)$. It will turn out that formula (2.2) holds for continuous functions ψ with larger support than required in lemma 2.7. We need the following lemma, which will be proved in §2.4.

<u>LEMMA 2.8</u>. *Let* K *be an open cube* $\{y \in \mathbb{R}^n \mid |y^i - y_0^i| < a,\ i = 1,\dots,n\}$ *such that* $\bar{K} \subset \mathbb{R}^n - f(\partial\Omega)$. *Let* $\psi\colon \mathbb{R}^n \to \mathbb{R}$ *be a continuous function vanishing outside* $\bar{K}$ *and let* $\int_{\mathbb{R}^n} \psi(y)dy = 0$. *Then*

$$\int_\Omega \psi(f(x))J_f(x)dx = 0. \tag{2.3}$$

Lemmas 2.8 and 2.7 immediately imply:

COROLLARY 2.9. *Let* $K \subset \mathbb{R}^n$ *be an open cube such that* $\bar{K} \subset \mathbb{R}^n - f(\partial\Omega)$. *Then for all continuous functions* $\psi\colon \mathbb{R}^n \to \mathbb{R}$ *vanishing outside* $\bar{K}$ *and such that* $\int_{\mathbb{R}^n} \psi(y)dy = 1$ *the integral*

$$\int_\Omega \psi(f(x))J_f(x)dx$$

has the same value. In particular, if $p \in K \cap (\mathbb{R}^n - f(Z))$ *then this integral is equal to* $\deg(f,\Omega,p)$.

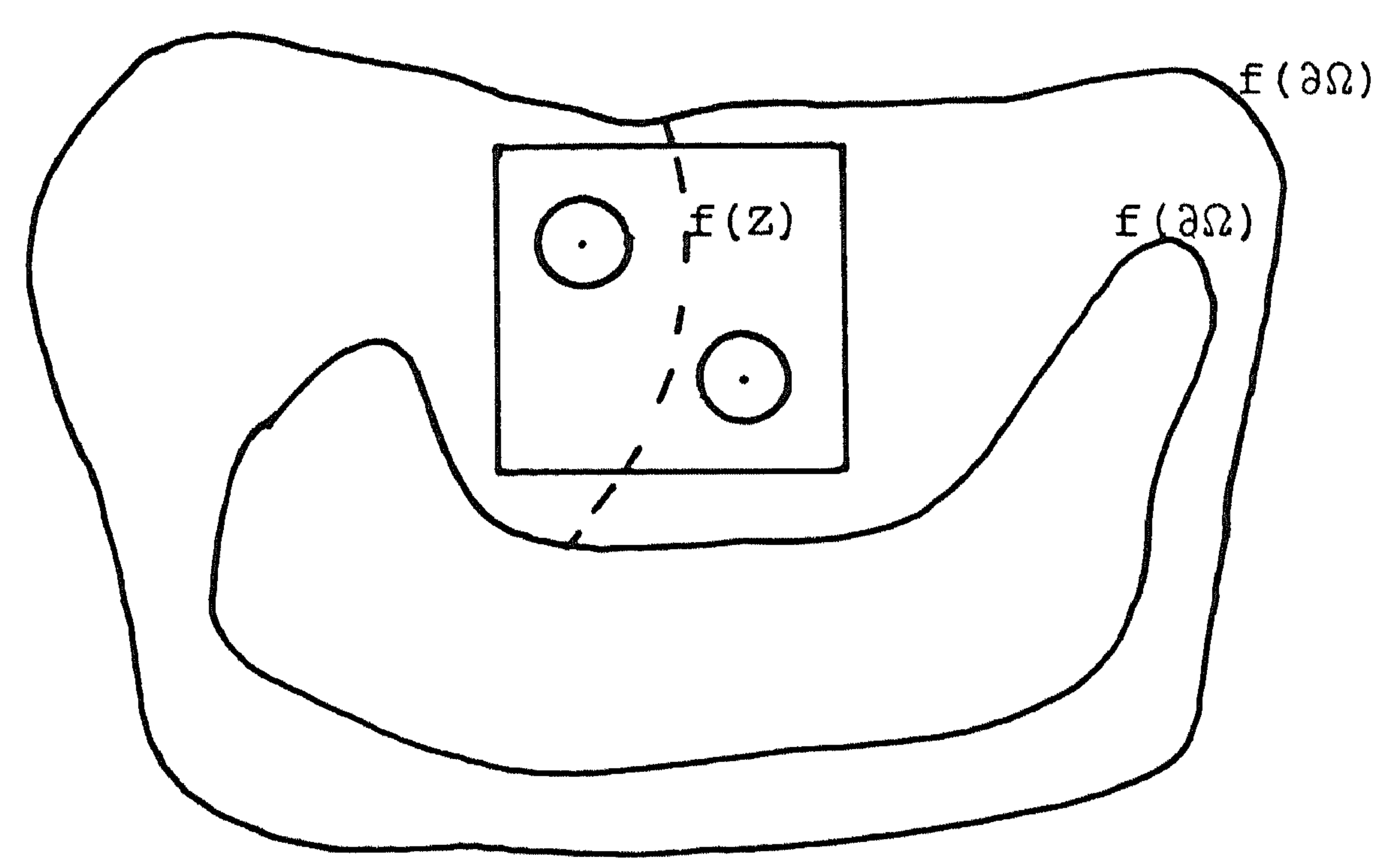

Figure 9

It follows that $\deg(f,\Omega,p)$ has the same value for all regular values p in any open cube with closure in $\mathbb{R}^n - f(\partial\Omega)$. It is now obvious how to extend the definition of degree to critical values $p \in \mathbb{R}^n - f(\partial\Omega)$.

DEFINITION 2.10. Let $f \in C(\bar{\Omega}) \cap C^1(\Omega)$ and $p \in \mathbb{R}^n - f(\partial\Omega)$. Let $K \subset \mathbb{R}^n$ be an open cube such that $p \in K$ and $\bar{K} \subset \mathbb{R}^n - f(\partial\Omega)$. Let $q \in K - f(Z)$ and let $\deg(f,\Omega,q)$ be given by (2.1). Then we define

$$\deg(f,\Omega,p) = \deg(f,\Omega,q).$$

This definition is independent of the choice of K and q and it is consistent with definition 2.4. It follows that $\deg(f,\Omega,p)$ is a locally constant integer-valued function of p on $\mathbb{R}^n - f(\partial\Omega)$. Clearly, $\deg(f,\Omega,p)$ is continuous in p.

COROLLARY 2.11. *Let* $f \in C(\bar{\Omega}) \cap C^1(\Omega)$. *Then* $\deg(f,\Omega,p)$ *is a constant function of* p *on each connected component of* $\mathbb{R}^n - f(\partial\Omega)$. *In particular,* $\deg(f,\Omega,p) = 0$ *on the unbounded connected component of* $\mathbb{R}^n - f(\partial\Omega)$.

If V is a connected component of $\mathbb{R}^n - f(\partial\Omega)$ and if $p \in V$ then we may write $\deg(f,\Omega,V)$ instead of $\deg(f,\Omega,p)$. NIRENBERG [8, theorem 1.5.5] proved the following integral representation for $\deg(f,\Omega,V)$.

THEOREM 2.12. *Let* $f \in C(\bar{\Omega}) \cap C^1(\Omega)$ *and let* V *be a connected component of* $\mathbb{R}^n - f(\partial\Omega)$. *Let* $\psi\colon \mathbb{R}^n \to \mathbb{R}$ *be a continuous function with compact support in* V *and let* $\int_{\mathbb{R}^n} \psi(y)\,dy = 1$. *Then*

$$\deg(f,\Omega,V) = \int_\Omega \psi(f(x))J_f(x)\,dx. \tag{2.4}$$

A proof will be given in §2.4.

2.3. THIRD STAGE: EXTENSION TO CONTINUOUS FUNCTIONS f

In §2.2 we proved that $\deg(f,\Omega,p)$ is a locally constant function of p. We shall now prove that, in a certain sense, $\deg(f,\Omega,p)$ is a locally constant function of f.

LEMMA 2.13. *Let* $f_0, f_1 \in C(\bar{\Omega}) \cap C^1(\Omega)$. *Define for* $0 \le t \le 1$ $f_t = tf_1 + (1-t)f_0$. *Suppose that* $p \notin f_t(\partial\Omega)$ *if* $0 \le t \le 1$. *Then* $\deg(f_t,\Omega,p)$ *is independent of* t.

PROOF. Since the mapping $(x,t) \to f_t(x)$ is continuous and the set $\partial\Omega \times [0,1]$ is compact, the set $\{f_t(x) \mid x \in \partial\Omega,\ 0 \le t \le 1\}$ is also compact. Hence, there is an open cube K such that $p \in K$ and $\bar{K} \subset \mathbb{R}^n - f_t(\partial\Omega)$ for all $t \in [0,1]$. Choose a continuous function $\psi\colon \mathbb{R}^n \to \mathbb{R}$ with support in K such that $\int_{\mathbb{R}^n} \psi(y)\,dy = 1$. Then

$$\deg(f_t,\Omega,p) = \int_\Omega \psi(f_t(x))(tJ_{f_1}(x)+(1-t)J_{f_0}(x))\,dx. \tag{2.5}$$

Since the function $(x,t) \to \psi(f_t(x))$ is uniformly continuous on the compact set $\bar{\Omega} \times [0,1]$, the right-hand side of (2.5) is continuous in t. Finally, since $\deg(f_t,\Omega,p)$ is integer-valued and continuous in t, it must be independent of t. □

COROLLARY 2.14. *Let* $p \in \mathbb{R}^n$. *Let* V *be a convex subset of* $C(\bar{\Omega})$ *such that* $p \notin f(\partial\Omega)$ *for each* $f \in V$. *Then* $\deg(f,\Omega,p)$ *has the same value for each* $f \in V \cap C^1(\Omega)$.

We are now able to give the third and final stage of the definition of degree.

DEFINITION 2.15. Let $f \in C(\bar{\Omega})$ and $p \in \mathbb{R}^n - f(\partial\Omega)$. Choose $r > 0$ such that $|y - p| > r$ for $y \in f(\partial\Omega)$. Let

$$V = \{g \in C(\bar{\Omega}) \mid \max_{x \in \bar{\Omega}} |g(x) - f(x)| < r\}.$$

Choose $g \in V \cap C^1(\Omega)$. Let $\deg(g,\Omega,p)$ be given by definition 2.10. Then we define

$$\deg(f,\Omega,p) = \deg(g,\Omega,p).$$

This definition is independent of the choice of r and g and it is consistent with definition 2.10. The degree $\deg(f,\Omega,p)$ considered as a function of $f \in C(\bar{\Omega})$ is integer-valued and locally constant with respect to the uniform topology on $C(\bar{\Omega})$.

2.4. APPENDIX

In this subsection proofs will be given for lemma 2.5, lemma 2.8 and theorem 2.12.

PROOF OF LEMMA 2.5. Since Ω is a countable union of closed cubes it suffices to consider a closed cube $K_0 \subset \Omega$ and to prove that $f(K_0 \cap Z)$ has Lebesgue measure zero. Suppose that K_0 has length ℓ. Let

$$M = \max_{x \in K_0} \left(\sum_{i,j=1}^{n} \left(\frac{\partial f^i(x)}{\partial x^j} \right)^2 \right)^{\frac{1}{2}}$$

Let $\varepsilon > 0$. Choose δ such that

$$\left(\sum_{i,j=1}^{n} \left(\frac{\partial f^i(x)}{\partial x^j} - \frac{\partial f^i(y)}{\partial x^j} \right)^2 \right)^{\frac{1}{2}} < \varepsilon$$

if $x,y \in K_0$ and $|x - y| < \delta$. Choose a natural number N such that $n^{\frac{1}{2}} N^{-1} \ell < \delta$. Subdivide the cube K_0 into N^n equal pieces by dividing each edge into N pieces. Consider a closed subcube K obtained in this way. Suppose that K

contains a critical point x_0. Then there is an orthogonal transformation $T\colon \mathbb{R}^n \to \mathbb{R}^n$ such that if $T \circ f = g$ then $\operatorname{grad} g^n(x_0) = 0$. For each $x \in K$ there are points $\xi_1,\xi_2,\ldots,\xi_n$ on the segment connecting x with x_0 such that

$$g^i(x) - g^i(x_0) = (\operatorname{grad} g^i(\xi_i), x-x_0), \qquad i = 1,\ldots,n.$$

Hence

$$|g^i(x) - g^i(x_0)| \le Mn^{\frac{1}{2}}N^{-1}\ell, \qquad i = 1,\ldots,n-1.$$

$$|g^n(x) - g^n(x_0)| \le \varepsilon n^{\frac{1}{2}}N^{-1}\ell.$$

Thus the measure of $f(K)$ is less than $\varepsilon M^{n-1}2^n n^{n/2}\ell^n N^{-n}$ and the measure of $f(K_0 \cap Z)$ is less than $\varepsilon M^{n-1}2^n n^{n/2}\ell^n$. Since ε is arbitrary, it follows that $f(K_0 \cap Z)$ has measure zero. □

Next we shall prove lemma 2.8. Some further lemmas will be needed.

<u>LEMMA 2.16</u>. *Let* K *be a closed cube in* $\mathbb{R}^n$. *Let* $\psi\colon \mathbb{R}^n \to \mathbb{R}$ *be a* C^1*-function with support in* K *such that* $\int_{\mathbb{R}^n} \psi(y)dy = 0$. *Then there exists a* C^1*-mapping* $v\colon \mathbb{R}^n \to \mathbb{R}^n$ *with support in* K *such that* $\operatorname{div} v = \psi$.

<u>PROOF</u>. The proof is by induction on the dimension n. When $n = 1$, the function $v(y) = \int_{-\infty}^{y} \psi(s)ds$ satisfies the conditions. Now suppose the lemma is true in n dimensions. We want to prove it in $n + 1$ dimensions. Without losing generality we may suppose that $K = K_{n+1} = \{y \in \mathbb{R}^{n+1} \mid |y^i| \le 1,\ i = 1,\ldots,n+1\}$. Let $K_n = \{y \in \mathbb{R}^n \mid |y^i| \le 1,\ i = 1,\ldots,n\}$. Let $\psi\colon \mathbb{R}^{n+1} \to \mathbb{R}$ be of class C^1 with support in K_{n+1} such that $\int_{\mathbb{R}^{n+1}} \psi(y)dy = 0$. Define a C^1-function $\phi\colon \mathbb{R}^n \to \mathbb{R}$ with support in K_n by

$$\phi(y) = \int_{-\infty}^{\infty} \psi(y,t)dt, \qquad y \in \mathbb{R}^n.$$

Then $\int_{\mathbb{R}^n} \phi(y)dy = 0$. By induction there is a C^1-mapping $u\colon \mathbb{R}^n \to \mathbb{R}^n$ with support in K_n such that $\operatorname{div} u = \phi$. Choose a C^1-function $\tau\colon \mathbb{R} \to \mathbb{R}$ with support in $[-1,1]$ such that $\int_{-\infty}^{\infty} \tau(t)dt = 1$. Then

$$\int_{-\infty}^{\infty} (\psi(y,t) - \phi(y)\tau(t))dt = 0, \qquad y \in \mathbb{R}^n.$$

Define a C^1-function $v^{n+1}\colon \mathbb{R}^{n+1} \to \mathbb{R}$ with support in K_{n+1} by

$$v^{n+1}(y,t) = \int_{-\infty}^{t} (\psi(y,s) - \phi(y)\tau(s))ds, \qquad (y,t) \in \mathbb{R}^n \times \mathbb{R}.$$

Then

$$\frac{\partial v^{n+1}(y,t)}{\partial t} = \psi(y,t) - \phi(y)\tau(t) = \psi(y,t) - \sum_{i=1}^{n} \frac{\partial}{\partial y^i}(u^i(y)\tau(t)).$$

By putting $v^i(y,t) = u^i(y)\tau(t)$, $i = 1,\dots,n$, the mapping $v = (v^1,\dots,v^{n+1})$ satisfies the conditions. □

If $f\colon \Omega \to \mathbb{R}^n$ is a C^1-mapping then let $J_f^{ij}(x)$ denote the cofactor corresponding to the (i,j)-th entry in the Jacobian matrix $(\frac{\partial f^i(x)}{\partial x^j})$. The formula

$$(2.6) \qquad \sum_{k=1}^{n} \frac{\partial f^\ell(x)}{\partial x^k} J_f^{ik}(x) = \delta_{i\ell} J_f(x)$$

is a standard result from linear algebra. We also have the following result.

<u>LEMMA 2.17</u>. *If* $f\colon \Omega \to \mathbb{R}^n$ *is a* C^2*-mapping then*

$$(2.7) \qquad \sum_{k=1}^{n} \frac{\partial J_f^{ik}(x)}{\partial x^k} = 0, \qquad i = 1,\dots,n.$$

<u>PROOF</u>. Fix i and write $g = (-1)^{i-1}(f^1,\dots,\hat{f}^i,\dots,f^n)$, where $\wedge$ denotes an absent element. Then

$$J_f^{ik}(x) = (-1)^{k-1}\det\left\{\frac{\partial g}{\partial x^1},\dots,\widehat{\frac{\partial g}{\partial x^k}},\dots,\frac{\partial g}{\partial x^n}\right\}.$$

Hence

$$\sum_{k=1}^{n} \frac{\partial J_f^{ik}(x)}{\partial x^k} = \sum_{k\neq\ell} (-1)^{k-1}\det\left\{\frac{\partial g}{\partial x^1},\dots,\frac{\partial^2 g}{\partial x^k \partial x^\ell},\dots,\widehat{\frac{\partial g}{\partial x^k}},\dots,\frac{\partial g}{\partial x^n}\right\} =$$

$$= \sum_{\ell<k} (-1)^{k+\ell-2}\det\left\{\frac{\partial^2 g}{\partial x^k \partial x^\ell},\frac{\partial g}{\partial x^1},\dots,\widehat{\frac{\partial g}{\partial x^\ell}},\dots,\widehat{\frac{\partial g}{\partial x^k}},\dots,\frac{\partial g}{\partial x^n}\right\} +$$

$$+ \sum_{\ell>k} (-1)^{k+\ell-3}\det\left\{\frac{\partial^2 g}{\partial x^k \partial x^\ell},\frac{\partial g}{\partial x^1},\dots,\widehat{\frac{\partial g}{\partial x^k}},\dots,\widehat{\frac{\partial g}{\partial x^\ell}},\dots,\frac{\partial g}{\partial x^n}\right\} =$$

$$= 0.$$ □

<u>LEMMA 2.18</u>. *Let* K, ψ *and* v *be as in Lemma* 2.16. *Let* $f\colon \bar{\Omega} \to \mathbb{R}^n$ *be of class* $C(\bar{\Omega}) \cap C^2(\Omega)$. *Let* $K \subset \mathbb{R}^n - f(\partial\Omega)$. *Then there is a* C^1*-mapping* $u\colon \mathbb{R}^n \to \mathbb{R}^n$ *with compact support in* Ω *such that*

$$\psi(f(x))J_f(x) = \operatorname{div} u(x), \qquad x \in \Omega.$$

PROOF. Define for $i = 1,\dots,n$

$$u^i(x) = \begin{cases} \sum_{k=1}^{n} v^k(f(x))J_f^{ki}(x) & \text{if } x \in \Omega, \\ 0 & \text{if } x \notin \Omega. \end{cases}$$

Then the mapping $u\colon \mathbb{R}^n \to \mathbb{R}^n$ is of class C^1 with support in the compact set $f^{-1}(K) \subset \Omega$. Using (2.6) and (2.7) we have

$$\begin{aligned} \operatorname{div} u(x) &= \sum_{i,k,\ell=1}^{n} \left[\frac{\partial v^k(y)}{\partial y^\ell}\right]_{y=f(x)} \frac{\partial f^\ell(x)}{\partial x^i} J_f^{ki}(x) + \\ &+ \sum_{i,k=1}^{n} v^k(f(x)) \frac{\partial J_f^{ki}(x)}{\partial x^i} = [\operatorname{div} v(y)]_{y=f(x)} J_f(x) = \\ &= \psi(f(x))J_f(x). \qquad \square \end{aligned}$$

REMARK 2.19. Lemmas 2.16 and 2.18 can also be formulated in terms of differential forms, cf. NIRENBERG [8, §1.3]. Consider a differential n-form $\mu = \psi(y)dy^{-1}\dots dy^n$ and a differential (n-1)-form $\omega = \sum_{i=1}^n (-1)^{i-1}v^i(y)dy^1\dots$ $\dots d\hat{y}{}^i\dots dy^n$. Then $\mu = d\omega$ if and only if $\psi(y) = \operatorname{div} v(y)$. Lemma 2.16 states that if μ is of class C^1 with support in K then there exists a (n-1)-form ω with support in K such that $\mu = d\omega$. The C^2-mapping $f\colon \Omega \to \mathbb{R}^n$ induces a mapping f^* from differential forms on $\mathbb{R}^n$ to differential forms on Ω. Lemma 2.18 is equivalent with the statement that $f^*(d\omega) = d(f^*\omega)$.

LEMMA 2.20. *Let $u\colon \mathbb{R}^n \to \mathbb{R}^n$ be mapping with compact support in Ω. Then*

$$\int_\Omega \operatorname{div} u(x)dx = 0.$$

PROOF. Apply Stokes' theorem. $\square$

Lemmas 2.16, 2.18 and 2.20 together imply:

COROLLARY 2.21. *Lemma 2.8 is valid if ψ is a C^1-function and* $f \in C(\bar\Omega) \cap C^2(\Omega)$.

PROOF OF LEMMA 2.8. Let the mapping $f \in C(\bar\Omega) \cap C^1(\Omega)$, the open cube K and the continuous function ψ be as in lemma 2.8. Let K_0 be an open cube in $\mathbb{R}^n$ such that $\bar K \subset K_0 \subset \bar K_0 \subset \mathbb{R}^n - f(\partial\Omega)$. Let U be an open set in Ω such that $f^{-1}(\bar K_0) \subset U \subset \bar U \subset \Omega$. It is possible to choose a mapping $g \in C(\bar\Omega) \cap C^2(\Omega)$

and a C^1-function ϕ such that $\bar{K}_0 \subset \mathbb{R}^n - g(\partial\Omega)$, $g^{-1}(\bar{K}_0) \subset U$, ϕ has support in K_0, $\int_{\mathbb{R}^n} \phi(y)dy = 0$, and such that the $C(\mathbb{R}^n)$-norm of $\psi - \phi$ and the $(C(\bar{\Omega}) \cap C^1(U))$-norm of $f - g$ are arbitrarily small, cf. for instance DEIMLING [9, p.25, Satz 2]. Now we have

$$\int_\Omega \psi(f(x))J_f(x)dx = \int_U (\psi(f(x)) - \psi(g(x)))J_f(x)dx +$$

$$+ \int_U (\psi(g(x)) - \phi(g(x)))J_f(x)dx +$$

$$+ \int_U \phi(g(x))(J_f(x) - J_g(x))dx + \int_\Omega \phi(g(x))J_g(x)dx.$$

The last term of the right-hand side is zero by corollary 2.21 and the other terms can be made arbitrarily small. Hence the left-hand side is zero. □

PROOF OF THEOREM 2.12. The open set V can be written as a countable union of open cubes K_α, such that each $y \in V$ has a neighborhood which intersects only finitely many of these cubes. For each cube K_α choose a continuous function $\phi_\alpha\colon \mathbb{R}^n \to \mathbb{R}$ with support in $\bar{K}_\alpha$ such that $\phi_\alpha(y) > 0$ if $y \in K_\alpha$. Let $\chi_\alpha(y) = \phi_\alpha(y)/(\Sigma_\beta\phi_\beta(y))$. Then $\chi_\alpha\colon V \to \mathbb{R}$ is well-defined, continuous and with support in $\bar{K}_\alpha$. Furthermore $\Sigma_\alpha\chi_\alpha(y) = 1$, $y \in V$ (partition of unity). It follows from corollary 2.9 that

$$\int_\Omega \psi(f(x))\chi_\alpha(f(x))J_f(x)dx = \deg(f,\Omega,V) \int_V \psi(y)\chi_\alpha(y)dy.$$

Summation over α then gives formula (2.4). □

3. PROPERTIES OF THE DEGREE

Let again Ω be an open bounded subset of $\mathbb{R}^n$, let $f: \bar{\Omega} \to \mathbb{R}^n$ be continuous and let $p \in \mathbb{R}^n - f(\partial\Omega)$. Let $\deg(f,\Omega,p)$ be defined by definition 2.15. For $g \in C(\bar{\Omega})$ let $\|g\| = \max_{x\in\bar{\Omega}} |g(x)|$. In this section we shall state some properties of the degree. In order to prove these properties the following proposition will be useful.

<u>PROPOSITION 3.1</u>. *Let* $0 < r \le \mathrm{dist}(p,f(\partial\Omega))$. *Let* $V = \{g \in C(\bar{\Omega}) \mid \|f-g\| < r\}$. *Then* $\deg(g,\Omega,p) = \deg(f,\Omega,p)$ *for each* $g \in V$ *and there exists* $g \in V \cap C^1(\Omega)$ *such that* p *is a regular value of* g.

<u>PROOF</u>. The first part of the proposition follows from corollary 2.14 and definition 2.15. To prove the second part we can choose $h \in V \cap C^1(\Omega)$ such that $\|h - f\| < \frac{1}{2}r$ (cf. lemma 2.6). Then by lemma 2.5 there is a regular value q of h such that $|q - p| < \frac{1}{2}r$. The mapping $g = h + p - q$ satisfies the conditions of the proposition. $\square$

Several properties of degree will follow by first approximating f by a mapping g as in proposition 3.1 and then applying formula (2.1). For instance, we can prove in this way that

$$\deg(f,\Omega,p) = \deg(f-p,\Omega,0). \tag{3.1}$$

The following important theorem can also be proved by this method.

<u>THEOREM 3.2</u>.
(a) *If* $f^{-1}(p)$ *is empty then* $\deg(f,\Omega,p) = 0$.
(b) *If* $\deg(f,\Omega,p) \ne 0$ *then* $f(x) = p$ *has at least one solution in* Ω.

<u>PROOF of (a)</u>. Let $f^{-1}(p) = \emptyset$. Choose $g \in C(\bar{\Omega}) \cap C^1(\Omega)$ such that $\|g - f\| < \mathrm{dist}(p,f(\bar{\Omega}))$ and p is a regular value of g. Then $g^{-1}(p) = \emptyset$ and $\deg(g,\Omega,p) = 0$ by (2.1). Hence $\deg(f,\Omega,p) = 0$. $\square$

Proposition 3.1 and formula (3.1) together imply that $\deg(f,\Omega,p)$ is a locally constant function of p. Hence, corollary 2.11 is valid for each $f \in C(\bar{\Omega})$.

THEOREM 3.3. *Let* $f \in C(\bar{\Omega})$. *Then* $\deg(f,\Omega,p)$ *is a constant function of* p *on each connected component of* $\mathbb{R}^n - f(\partial\Omega)$. *If* V *is such a component containing a point* p *for which* $f^{-1}(p) = \emptyset$ *then* $\deg(f,\Omega,V) = 0$. *In particular,* $\deg(f,\Omega,V) = 0$ *if* V *is the unbounded component of* $\mathbb{R}^n - f(\partial\Omega)$.

The first part of proposition 3.1 is equivalent with:

THEOREM 3.4. *(Homotopy invariance)*
Let the mapping $(x,t) \to f_t(x)$ *be continuous from* $\bar{\Omega} \times [0,1]$ *into* $\mathbb{R}^n$ *and let* $f_t(x) \neq p$ *if* $(x,t) \in \partial\Omega \times [0,1]$. *Then* $\deg(f_t,\Omega,p)$ *is independent of* t.

For linear mappings f formula (2.1) reduces to:

THEOREM 3.5. *Let* $A\colon \mathbb{R}^n \to \mathbb{R}^n$ *be a nonsingular linear transformation, let* $b \in \mathbb{R}^n$, $f(x) = Ax + b$ *and* $p \in f(\Omega)$. *Then* $\deg(f,\Omega,p) = \text{sign}\det A$.

The two following theorems describe the dependence of the degree on the domain Ω.

THEOREM 3.6. *(Excision property)*
Let $p \notin f(\partial\Omega)$, *let* K *be a closed subset of* $\bar{\Omega}$ *and let* $p \notin f(K)$. *Then*

$$\deg(f,\Omega,p) = \deg(f,\Omega-K,p)$$

PROOF. Let $p \notin f(K) \cup f(\partial\Omega)$. Choose $q \in C(\bar{\Omega}) \cap C^1(\Omega)$ such that $\|g - f\| < \text{dist}(p,f(K) \cup f(\partial\Omega))$ and p is a regular value of g. Then by (2.1) and proposition 3.1 we have

$$\deg(f,\Omega,p) = \deg(g,\Omega,p) = \sum_{x\in g^{-1}(p)} \text{sign}\, J_g(x) =$$

$$= \sum_{x\in g^{-1}(p)-K} \text{sign}\, J_g(x) = \deg(g,\Omega-K,p) = \deg(f,\Omega-K,p).$$

$\square$

<u>THEOREM 3.7</u>. (*Domain decomposition*)
Let $p \notin f(\partial\Omega)$. *If* Ω *is a countable union of disjoint open sets* Ω_j *then*

$$\deg(f,\Omega,p) = \sum_j \deg(f,\Omega_j,p). \tag{3.2}$$

On the right only a finite number of terms are nonzero.

<u>PROOF</u>. First we prove that $p \notin \partial\Omega_j$ for each j. Suppose that $p \in \partial\Omega_k$ for some k. Then $p \in \bar{\Omega}$, $p \notin \partial\Omega$, so $p \in \Omega$. Hence $p \in \Omega_\ell$ for some ℓ, $\ell \neq k$. It follows that $p \in \partial\Omega_k$ is an interior point of Ω_ℓ. Hence $\Omega_k \cap \Omega_\ell \neq \emptyset$. This is a contradiction.

Next choose $g \in C(\bar{\Omega}) \cap C^1(\Omega)$ such that $\|g - f\| < \mathrm{dist}(p,f(\partial\Omega))$ and p is a regular value of g. Then $\deg(f,\Omega,p) = \deg(g,\Omega,p)$ and $\deg(f,\Omega_j,p) = \deg(g,\Omega_j,p)$ for each j. Since $g^{-1}(p)$ is a finite set, $\deg(g,\Omega_j,p) = 0$ for all but finitely many values of j. Finally, (2.1) implies (3.2) with f replaced by g. Therefore (3.2) also holds for f. □

<u>REMARK 3.8</u>. The reader may verify that theorems 3.4, 3.5, 3.6, 3.7 together imply definition 2.4 and that theorem 3.4 and definition 2.4 together imply definition 2.15. Hence, the degree is completely characterized by theorems 3.4, 3.5, 3.6 and 3.7.

<u>THEOREM 3.9</u>. (*Boundary value dependence*)
For fixed Ω *and* p *the degree* $\deg(f,\Omega,p)$ *is completely determined by the restriction of* f *to* $\partial\Omega$.

<u>PROOF</u>. Let $f_0,f_1 \in C(\bar{\Omega})$. Suppose that $f_0(x) = f_1(x)$ for $x \in \partial\Omega$. Let $p \notin f_0(\partial\Omega)$. Define $f_t = tf_1 + (1-t)f_0$. Then $f_0 = f_t = f_1$ on $\partial\Omega$. Theorem 3.4 implies that

$$\deg(f_0,\Omega,p) = \deg(f_1,\Omega,p). \qquad \square$$

<u>REMARK 3.10</u>. It follows from the *Tietze extension theorem* (cf. for instance SIMMONS [10, §28]) and from the compactness of $\partial\Omega$ that each continuous mapping $h\colon \partial\Omega \to \mathbb{R}^n$ has a *continuous extension* f to $\bar{\Omega}$. This observation together with theorem 3.9 makes it possible to define the degree $\deg(h,\partial\Omega,p)$ if $h\colon \partial\Omega \to \mathbb{R}^n$ is a continuous mapping and $p \notin h(\partial\Omega)$. Choose any continuous extension f of h on $\bar{\Omega}$ and define $\deg(h,\partial\Omega,p) = \deg(f,\Omega,p)$.

Theorem 3.4 already holds for homotopy equivalence on the boundary.

THEOREM 3.11. *Let* $f_0, f_1 \colon \bar{\Omega} \to \mathbb{R}^n$ *be continuous mappings. Suppose that there exist mappings* $f_t \colon \partial\Omega \to \mathbb{R}^n$, $0 < t < 1$, *such that the mapping* $(x,t) \to f_t(x)$ *is continuous from* $\partial\Omega \times [0,1]$ *into* $\mathbb{R}^n$ *and* $f_t(x) \neq p$ *if* $(x,t) \in \partial\Omega \times [0,1]$. *Then* $\deg(f_0,\Omega,p) = \deg(f_1,\Omega,p)$.

PROOF. The mapping $(x,t) \to f_t(x)$ is continuous on the compact set $(\bar{\Omega} \times \{0\}) \cup (\partial\Omega \times [0,1]) \cup (\bar{\Omega} \times \{1\})$. By the Tietze extension theorem it has a continuous extension on $\bar{\Omega} \times [0,1]$. Application of theorem 3.4 completes the proof. □

Finally we define the index of an isolated solution of $f(x) = p$.

DEFINITION 3.12. Let $f \colon \bar{\Omega} \to \mathbb{R}^n$ be continuous. Let $p \in \mathbb{R}^n$. If $x \in \Omega$ is an isolated point of $f^{-1}(p)$ then define the *index* of f relative to p at the point x by

$$\operatorname{ind}(f,x,p) = \deg(f,B_r(x),p), \tag{3.3}$$

where $B_r(x)$ is an open ball of radius r around x such that $B_r(x) \subset \Omega$ and $f^{-1}(p) \cap B_r(x) = \{x\}$.

Theorem 3.6 guarantees that this definition does not depend on the choice of r.

THEOREM 3.13. *Let* $f \in C(\bar{\Omega}) \cap C^1(\Omega)$ *and* $p \in \mathbb{R}^n$. *If* $x \in \Omega$ *is an isolated point of* $f^{-1}(p)$ *and if* $J_f(x) \neq 0$ *then*

$$\operatorname{ind}(f,x,p) = \operatorname{sign} J_f(x) = (-1)^{\nu}, \tag{3.4}$$

where ν *is the sum of the algebraic multiplicities of the real negative eigenvalues of the Jacobian of* f *in* x.

PROOF. The first equality follows from (2.1) and (3.3). Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the Jacobian of f in x. Then $J_f(x) = \lambda_1\lambda_2\ldots\lambda_n$. The nonreal factors occur in complex conjugate pairs. Hence only the real negative factors contribute to the sign. □

Note that if $J_f(x) = 0$ then the index of f at x can assume integral values different from -1 or 1.

THEOREM 3.14. *Let* $f \in C(\bar{\Omega})$. *If* $f^{-1}(p)$ *is a finite set included in* Ω *then*

$$\deg(f,\Omega,p) = \sum_{x\in f^{-1}(p)} \operatorname{ind}(f,x,p). \tag{3.5}$$

PROOF. Let $f^{-1}(p) = \{x_1,x_2,\dots,x_k\}$. Choose disjoint open balls $B_{r_j}(x_j) \subset \Omega$, $j = 1,\dots,k$. Application of theorems 3.6 and 3.7 gives

$$\deg(f,\Omega,p) = \deg\left(f, \bigcup_{j=1}^{k} B_{r_j}(x_j),p\right) = \sum_{j=1}^{k} \deg(f,B_{r_j}(x_j)p) =$$

$$= \sum_{x\in f^{-1}(p)} \operatorname{ind}(f,x,p). \qquad \square$$

4. SOME APPLICATIONS TO NONLINEAR EQUATIONS

In this section we shall discuss Brouwer's fixed point theorem, a theorem about the surjectivity of a mapping, and the existence of eigenvalues for certain nonlinear mappings. The homotopy invariance theorems 3.4 and 3.11 will be the main tools for proving these theorems. Throughout, the reader may consult the references [5] - [9]. In addition, SMART [11, chaps. 2 and 10] is a good reference for fixed point theorems.

4.1. BROUWER'S FIXED POINT THEOREM

Let B^n denote the closed unit ball in $\mathbb{R}^n$ and let $S^{n-1} = \partial B^n$ be the unit sphere in $\mathbb{R}^n$. Remember that a topological space X has the *fixed point property* if for each continuous mapping $f: X \to X$ there exists a (fixed) point x in X such that $f(x) = x$.

THEOREM 4.1. (BROUWER)
The closed unit ball B^n has the fixed point property.

PROOF. Suppose that $f: B^n \to B^n$ is continuous without fixed points. Let $g(x) = x - f(x)$. Then the equation $g(x) = 0$ has no solutions. Define $g_t(x) = x - (1-t)f(x)$. Then $(x,t) \to g_t(x)$ is continuous from $B^n \times [0,1]$ into $\mathbb{R}^n$, $g_0 = g$, $g_1 = \mathrm{id}$ and $g_t(x) \neq 0$ if $(x,t) \in S^{n-1} \times [0,1]$. Application of theorems 3.2, 3.4 and 3.5 gives

$$0 = \deg(g, B^n - S^{n-1}, 0) = \deg(\mathrm{id}, B^n - S^{n-1}, 0) = 1.$$

This is a contradiction. □

Without using any degree theory it can easily be proved that the following two propositions are equivalent with theorem 4.1.

PROPOSITION 4.2. (S^{n-1} *is not contractible*)
There does not exist a continuous mapping $(x,t) \to f_t(x)$ *from* $S^{n-1} \times [0,1]$ *to* S^{n-1} *such that* f_1 *is the identity mapping and* f_0 *maps* S^{n-1} *onto one point.*

PROPOSITION 4.3. (S^{n-1} *is not a retract of* B^n)
There does not exist a continuous mapping $g: B^n \to S^{n-1}$ *such that* $g|_{S^{n-1}}$ *is the identity mapping.*

PROOF that proposition 4.3 implies theorem 4.1.
Suppose that $f: B^n \to B^n$ is a continuous mapping without fixed points. Then for each $x \in B^n$ there exists a unique real number $t \geq 1$ such that the point $tx + (1-t)f(x)$ lies in S^{n-1}. Denote this point by $g(x)$. Then the mapping $g: B^n \to S^{n-1}$ is continuous and $g|_{S^{n-1}} = \mathrm{id}$. □

It is left to the reader to prove that theorem 4.1 implies proposition 4.3 and that propositions 4.2 and 4.3 imply each other.

It is evident from theorem 4.1 that each topological space which is homeomorphic with B^n, has the fixed point property.

LEMMA 4.4. *Any nonempty compact convex subset* K *of* $\mathbb{R}^n$ *is homeomorphic with some* B^m, $m \leq n$.

SKETCH OF THE PROOF. (See KANTOROVICH & AKILOV [12, p.638] for the details). Without losing generality we may suppose that $0 \in K$ and that $\mathbb{R}^n$ is the linear span of K. Then, by the convexity of K, the interior of K is open. Let the point 0 be in the interior of K. Now it is possible to define the Minkowski functional $p(x) = \inf\{t > 0 \mid t^{-1}x \in K\}$, $x \in \mathbb{R}^n$. Then the mapping g defined by $g(x) = (p(x))^{-1} |x| x$, $x \neq 0$, and $g(0) = 0$, is a homeomorphic mapping from B^n onto K. □

THEOREM 4.5. *Any nonempty compact convex subset of* $\mathbb{R}^n$ *has the fixed point property.*

The following proof of a result of FROBENIUS is a nice application of theorem 4.5.

THEOREM 4.6. (FROBENIUS)
Suppose A *is an* $n \times n$ *matrix* (a_{ij}) *with* $a_{ij} > 0$ *for* $i,j = 1,\dots,n$. *Then* A *has a positive eigenvalue and a corresponding eigenvector* $x = (x^1,\dots,x^n)$ *with all* $x^i \geq 0$.

PROOF. If $x \neq 0$ with all $x^i \geq 0$ then $y = Ax \neq 0$ with all $y^j \geq 0$. The mapping f defined by $f(x) = (\sum_{j=1}^n (Ax)^j)^{-1}Ax$ is continuous from the compact convex set $K = \{x \in \mathbb{R}^n \mid x^1 + \dots + x^n = 1,\ x^i \geq 0 \text{ for } i = 1,\dots,n\}$ into itself. Hence $f(x_0) = x_0$ for some $x_0 \in K$. Then $Ax_0 = (y_0^1+\dots+y_0^n)x_0 = \lambda x_0$ and $\lambda > 0$. □

4.2. ON THE SURJECTIVITY OF A MAPPING $f\colon \mathbb{R}^n \to \mathbb{R}^n$

PROPOSITION 4.7. *Let* $f\colon B^n \to \mathbb{R}^n$ *be continuous such that* $f(x)$ *never points opposite to* x *for* $x \in S^{n-1}$, *i.e.,* $f(x) \neq -\lambda x$ *for all* $\lambda \geq 0$, $x \in S^{n-1}$. *Then* $f(x) = 0$ *has a solution in the interior of* B^n.

PROOF. Let $f_t(x) = tf(x) + (1-t)x$, $0 \leq t \leq 1$. Then, by hypothesis, $f_t(x) \neq 0$ for $(x,t) \in S^{n-1} \times [0,1]$. Hence

$$\deg(f, B^n - S^{n-1}, 0) = \deg(\mathrm{id}, B^n - S^{n-1}, 0) = 1.$$

Application of theorem 3.2 completes the proof. □

In particular, the conditions of proposition 4.7 are satisfied if $(f(x),x) > 0$ for each $x \in S^{n-1}$.

PROPOSITION 4.8. *Let* $f\colon B^n \to \mathbb{R}^n$ *be continuous such that* $(f(x),x) \geq r$ *for some* $r > 0$ *and all* $x \in S^{n-1}$. *Then the equation* $f(x) = y$ *has a solution for each* y, $|y| < r$.

PROOF. Let $|y| < r$ and $g(x) = f(x) - y$. Then

$$(g(x),x) = (f(x),x) - (y,x) \geq r - |y| > 0, \qquad \text{for } x \in S^{n-1}.$$

Hence, by proposition 4.7, $g(x) = 0$ has a solution in B^n. □

THEOREM 4.9. *Let* $f\colon \mathbb{R}^n \to \mathbb{R}^n$ *be a continuous mapping. If*

$$|x|^{-1}(f(x),x) \to +\infty \text{ uniformly as } |x| \to \infty,$$

then f *is a surjection, i.e., for each* $y \in \mathbb{R}^n$ *the equation* $f(x) = y$ *has a solution.*

PROOF. Choose $r > 0$. Then, by hypothesis, there exists $R > 0$ such that $|x|^{-1}(f(x),x) \geq r$ for $|x| = R$. Define $g(x) = f(Rx)$. Then $(g(x),x) \geq r$ for $|x| = 1$. Hence, proposition 4.8 assures that $g(x) = y$, $y < r$, has solutions in B^n. So $f(x) = y$, $y < r$, has solutions for $|x| \leq R$. □

4.3. EIGENVALUES OF NONLINEAR MAPPINGS $f\colon S^{n-1} \to \mathbb{R}^n$

Theorem 3.9 and remark 3.10 justify the following definition.

DEFINITION 4.10. Let f: $S^{n-1} \to S^{n-1}$ be a continuous mapping. Then the *degree* deg(f) can be defined such that

$$\deg(f) = \deg(F, B^n - S^{n-1}, 0)$$

for any continuous extension $F: B^n \to \mathbb{R}^n$ of f.

Because of theorem 3.3 we have

$$\deg(f) = \deg(F, B^n - S^{n-1}, p)$$

for each $p \in B^n - S^{n-1}$. Application of theorem 3.11 gives:

PROPOSITION 4.11. (*Homotopy equivalence*)
If the continuous mappings $f_0, f_1: S^{n-1} \to S^{n-1}$ *are homotopic, i.e., if* f_0 *and* f_1 *can be extended to a continuous mapping* $(x,t) \to f_t(x)$ *from* $S^{n-1} \times [0,1]$ *into* S^{n-1}, *then* $\deg(f_0) = \deg(f_1)$.

LEMMA 4.12. *Let* $f: S^{n-1} \to S^{n-1}$ *be continuous.*
(a) *If* f *has no fixed point then* $\deg(f) = (-1)^n$.
(b) *If* $-f$ *has no fixed point then* $\deg(f) = 1$.

PROOF.
(a) Let $f_t(x) = |(1-t)f(x) - tx|^{-1}((1-t)f(x)-tx)$. Then $(x,t) \to f_t(x)$ is continuous from $S^{n-1} \times [0,1]$ into S^{n-1}, $f_0 = f$ and $f_1 = -\mathrm{id}$. Hence $\deg(f) = \deg(-\mathrm{id}) = (-1)^n$.
(b) Using the homotopy $f_t(x) = |(1-t)f(x) + tx|^{-1}((1-t)f(x)+tx)$ we obtain that $\deg(f) = \deg(\mathrm{id}) = 1$. □

COROLLARY 4.12. *Let* $f: S^{n-1} \to S^{n-1}$ *be continuous. If* n *is odd then either* f *or* $-f$ *has a fixed point.*

This result is a generalisation of the elementary fact that any orthogonal transformation of $\mathbb{R}^n$ must have eigenvalue 1 or -1 if n is odd.

THEOREM 4.13. *Let* $f: S^{n-1} \to \mathbb{R}^n$ *be continuous. If* n *is odd then there exists* $x_0 \in S^{n-1}$ *and* $\lambda \in \mathbb{R}$ *such that* $f(x_0) = \lambda x_0$.

PROOF. Clearly the theorem holds if $f(x) = 0$ for some $x \in S^{n-1}$. Suppose that f maps S^{n-1} into $\mathbb{R}^n - \{0\}$. Then $g = |f|^{-1}f$ is a continuous mapping from S^{n-1} into itself. By corollary 4.12 there exists $x_0 \in S^{n-1}$ and $\varepsilon = \pm 1$ such that $g(x_0) = \varepsilon x_0$. Hence $f(x_0) = \varepsilon |f(x_0)| x_0$. □

The linear case of this theorem states that for odd n any linear transformation A: $\mathbb{R}^n \to \mathbb{R}^n$ has a real eigenvalue.

COROLLARY 4.14. *Let* $f\colon S^{n-1} \to \mathbb{R}^n$ *be continuous and let* $(f(x),x) = 0$ *for each* $x \in S^{n-1}$. *If* n *is odd then* $f(x) = 0$ *for some* $x \in S^{n-1}$.

An equivalent statement is that for odd n any *tangent vector field* on S^{n-1} vanishes somewhere. The linear case of corollary 4.14 states that any linear skew-symmetric transformation A: $\mathbb{R}^n \to \mathbb{R}^n$ possesses an eigenvalue 0 if n is odd.

In corollaries 4.12, 4.14 and theorem 4.13 the condition that n is odd cannot be omitted. The reader may easily find counterexamples in the case that n is even.

5. SOME FURTHER PROPERTIES AND APPLICATIONS OF DEGREE

In this final section we mention some further interesting results without proofs.

5.1. DEGREE THEORY ON THE SPHERE

A theorem due to Hopf asserts that the converse of proposition 4.11 is true. Hence, the degree is essentially the only homotopy invariant for mappings from the sphere into itself.

THEOREM 5.1. (HOPF)
If $f_0, f_1\colon S^{n-1} \to S^{n-1}$ *are continuous and if* $\deg(f_0) = \deg(f_1)$ *then* f_0 *and* f_1 *are homotopic.*

The proof uses combinatorial topology, see HU [13, chap. 2, §8].

For mappings $f\colon S^{n-1} \to S^{n-1}$ the degree can also be defined without using the definition of degree for mappings $F\colon B^n \to \mathbb{R}^n$. Note that S^{n-1} is an (n-1)-dimensional *oriented differentiable manifold*. This means that S^{n-1} is a union of open subsets U_α with *local coordinates* $\xi_\alpha^1, \ldots, \xi_\alpha^{n-1}$ on each U_α such that on $U_\alpha \cap U_\beta$ ξ_α^i is a C^∞-function of $\xi_\beta^1, \ldots, \xi_\beta^{n-1}$ and $\det(\partial\xi_\alpha^i/\partial\xi_\beta^j) > 0$. Now the three stages of the analytic definition of degree (cf. section 2) can be repeated for mappings $f\colon S^{n-1} \to S^{n-1}$ and points p in S^{n-1}. All steps have to be done in terms of local coordinates and it has to be verified that things do not depend on the choice of the local coordinates. For further details about the analytic definition of degree for mappings between oriented manifolds we refer to NIRENBERG [8, chap. 1].

If $\deg(f, S^{n-1}, p)$, $p \in S^{n-1}$, is defined by the above method then this degree is a locally constant function of p. Hence, $\deg(f, S^{n-1}, p)$ has the same value for each $p \in S^{n-1}$, so the degree only depends on f. NIRENBERG [8, §1.5.7] proves that this definition of degree coincides with deg(f) in definition 4.10.

For mappings $f\colon B^n \to \mathbb{R}^n$ of class $C^1(B^n)$ (i.e. continuously differentiable also on the boundary of B^n) the degree can also be expressed by a *surface integral* due to Kronecker, cf. HADAMARD [14] and BERGER & BERGER [6, p.40]. Let $0 \notin f(S^{n-1})$. Then

$$(5.1) \qquad \deg(f, B^n - S^{n-1}, 0) = \frac{1}{K_{n-1}} \int_{S^{n-1}} |f|^{-n} \det\{f, \frac{\partial f}{\partial \xi^1}, \ldots, \frac{\partial f}{\partial \xi^{n-1}}\} d\xi^1 \ldots d\xi^{n-1},$$

where f has Cartesian coordinates $f^1,\dots,f^n$, where $\xi^1,\dots,\xi^{n-1}$ are suitable coordinates on S^{n-1} except for a subset of lower dimension, and where K_{n-1} is the surface area of S^{n-1}. Formula (5.1) is the n-dimensional analogue of (1.4) and (1.10).

The author of the present chapter obtained a proof of formula (5.1) as follows (unpublished). First define deg(f) for mappings $f\colon S^{n-1} \to S^{n-1}$ by using the differentiable manifold structure of S^{n-1}. Then formulate an analogue for deg(f) of the integral representation (2.4). Here ψ may have arbitrary support in S^{n-1}. Next, prove by some manipulation of determinants that deg(f) is equal to the right-hand side of (5.1) with $|f|^{-n} = 1$. Finally, replace f by $|f|^{-1}f$, where f is a mapping from B^n into $\mathbb{R}^n$.

5.2. THE MULTIPLICATIVE PROPERTY

THEOREM 5.2. *(Multiplication property)*
Let $\Omega \subset \mathbb{R}^n$ *be open and bounded. Let* $f\colon \bar{\Omega} \to \mathbb{R}^n$ *and* $g\colon \mathbb{R}^n \to \mathbb{R}^n$ *be continuous. Denote the bounded components of* $\mathbb{R}^n - f(\partial\Omega)$ *by* $V_1, V_2, \dots$ *. Suppose that* $p \notin g \circ f(\partial\Omega)$*. Then*

$$\deg(g\circ f,\Omega,p) = \sum_i \deg(f,\Omega,V_i)\,\deg(g,V_i,p),$$

where the sum on the right is finite.

This theorem as well as its two corollaries formulated below are proved in SCHWARTZ [5, pp.74-78] and HEINZ [4, §11].

COROLLARY 5.3. (JORDAN)
Let K *and* L *be homeomorphic compact sets in* $\mathbb{R}^n$. *If* $\mathbb{R}^n - K$ *has a finite number of components then* $\mathbb{R}^n - L$ *has the same number of components.*

In particular, if n = 2 and if K is the unit circle then L is an arbitrary *Jordan curve* and we obtain the well-known property that $\mathbb{R}^2 - L$ has two components.

COROLLARY 5.4. *(Domain invariance)*
Let U *be an open subset of* $\mathbb{R}^n$ *and let* $f\colon U \to \mathbb{R}^n$ *be a continuous one-to-one mapping. Then the image* f(U) *is open in* $\mathbb{R}^n$.

5.3. BORSUK'S THEOREM

For this subsection see SCHWARTZ [5, pp.78-82], NIRENBERG [8, §1.7] and DEIMLING [9, §10].

THEOREM 5.5. (BORSUK)
Let Ω *be a bounded open sbuset of* $\mathbb{R}^n$ *symmetric about the origin such that* $0 \in \Omega$. *Let* $f: \bar{\Omega} \to \mathbb{R}^n$ *be continuous such that* $f(x) = -f(-x) \neq 0$ *for all* $x \in \partial\Omega$. *Then* $\deg(f,\Omega,0)$ *is odd.*

COROLLARY 5.6. *Let* Ω *be as in theorem* 5.5. *Let* $f: \partial\Omega \to \mathbb{R}^n$ *be a continuous mapping whose image is contained in a* k*-dimensional subspace,* $k < n$, *of* $\mathbb{R}^n$.

(a) *There exists* $x \in \partial\Omega$ *such that* $f(x) = f(-x)$.

(b) *If* f *is an odd mapping then* $f(x) = 0$ *for some* $x \in \partial\Omega$.

COROLLARY 5.7. *Let* Ω *be as in theorem* 5.5. *Let* $A_1, A_2, \ldots, A_n$ *be* n *closed subsets of* $\partial\Omega$ *such that* $\partial\Omega = \bigcup_{i=1}^n A_i$. *Then at least one set* A_i *contains a pair of antipodal points* x *and* -x.

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III. CHEMICAL REACTIONS DESCRIBED BY AUTONOMOUS ORDINARY DIFFERENTIAL EQUATIONS

In this chapter we present some aspects of the theory of ordinary differential equations describing chemically reacting systems. The main topics are the a priori bounds of solutions and the existence and stability of equilibrium points, the latter aspect being considered by using degree theory developed in chapter II. As a general reference to the present chapter we mention the monograph of GAVALAS [1].

1. CHEMICAL REACTIONS

We consider a system of r simultaneous chemical reactions, symbolized by:

$$(1.1)\qquad \sum_{j=1}^{n} \nu_{ij}\, M_j = 0, \qquad i = 1,\ldots,r,$$

where ν_{ij} are integers and M_j are chemical species. The numbers ν_{ij} constitute an $(r\times n)$-matrix ν. The species M_j consists of a number of atomic species $A_1,\ldots,A_m$, and β_{ij} will denote the number of atoms A_j in the species M_i. The non-negative numbers β_{ij} constitute an $(n\times m)$-matrix β. Since each chemical species contains at least one atomic species we have

$$(1.2)\qquad \sum_{j=1}^{m} \beta_{ij} > 0, \qquad i = 1,\ldots,n$$

EXAMPLE 1.1. To illustrate the concepts in this section we shall consider the two reactions

$$(1.3)\qquad \begin{aligned} &2NO_2 - N_2O_4 = 0, \\ &2NO + O_2 - 2NO_2 = 0. \end{aligned}$$

The four chemical species O_2, NO, NO_2, N_2O_4 will be denoted by M_1, M_2, M_3, M_4 respectively, and the atomic species O, N are denoted by A_1 and A_2. The matrices ν and β are in this case

$$(1.4)\qquad \nu = \begin{pmatrix} 0 & 0 & 2 & -1 \\ 1 & 2 & -2 & 0 \end{pmatrix} \quad , \quad \beta = \begin{pmatrix} 2 & 0 \\ 1 & 1 \\ 2 & 1 \\ 4 & 2 \end{pmatrix}$$

REMARK 1.2. (Notation) The rank of a matrix α will be denoted by $r(\alpha)$ and the transpose of α by α^T. With I_n we denote the $(n\times n)$ unit matrix, and with 0_{nm} we denote the $(n\times m)$-matrix containing only zero elements.

REMARK 1.3. We suppose throughout that

$$(1.5)\qquad r(\nu) = r;$$

in other words, we only consider a system of r independent reactions. In general, the chemical equations are presented as $\sum \lambda_j M_j \overset{\leftarrow}{\rightarrow} \sum \mu_j M_j$ where the direction also is important, but in the mathematical treatment these aspects may be ignored.

REMARK 1.4. The r reactions (1.1) are said to be *proper* if

$$(1.6)\qquad \nu\beta = 0_{rm}.$$

The condition for a reaction to be proper is known in chemistry as "balancing the equations", and

$$(1.7)\qquad \sum_{j=1}^{n} \nu_{ij}\, \beta_{jk} = 0 \qquad (i=1,\ldots,r,\ k=1,\ldots,m)$$

corresponds to the conservation of atomic species A_k in the i-th reaction.

We only consider systems for which (1.6) is fulfilled.

The following lemma is important for the construction of invariant manifolds of the differential equations describing chemical reactions. It is an extension of relation (1.6).

LEMMA 1.5. *There is an* $n \times (n-r)$ *matrix* γ *of rank* $(n-r)$ *such that*

$$\nu\gamma = 0_{r,n-r}. \tag{1.8}$$

PROOF. The proof simply follows from the observation that the linear homogeneous equation $\nu x = 0$, $x \in \mathbb{R}^n$ has $(n-r)$ linearly independent solutions; here (1.5) is used. □

On account of (1.6) or (1.7), the first $r(\beta)$ columns of γ will be taken from the columns of β. If the elements of γ are denoted by γ_{ij}, then it follows from (1.2) that

$$p_i = \sum_{j=1}^{r(\beta)} \gamma_{ij} > 0, \qquad i = 1,\dots,n. \tag{1.9}$$

Moreover we have

$$r = r(\nu) \le n - r(\beta) \tag{1.10}$$

giving an upper bound for the number of linearly independent reactions.

It is supposed that the systems considered are *homogeneous*, that is, we suppose that only one phase in the system will occur. The concentration of the chemical species M_i will be denoted by c_i, $i=1,\dots,n$. During a reaction process the quantities c_i, which are called the *state variables*, will vary with time, and the evolution of a chemical system can be described by these variables as functions of time. The initial values (at t=0) are denoted by $c_{i0}, i = 1,\dots,n$. The state vector c and its initial value c_0

$$c = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix}, \qquad c_0 = \begin{pmatrix} c_{10} \\ \vdots \\ c_{n0} \end{pmatrix} \tag{1.11}$$

are the elements of the n-dimensional real vector space $\mathbb{R}^n$, and $\mathbb{R}^n_+$ is its positive orthant

$$(1.12) \qquad \mathbb{R}^n_+ = \{c \mid c_i \geq 0, \quad i = 1,\dots,n\}$$

The inner product $(.,.)$ and the norm $|.|$ in $\mathbb{R}^n$ are given by

$$(x,y) = x_1y_1 + \dots + x_ny_n, \quad |x| = (x,x)^{\frac{1}{2}}.$$

REMARK 1.6. If we interpret the r rows of ν as vectors of $\mathbb{R}^n$, the subspace spanned by these rows is denoted by Λ_0. On account of (1.5), dim $(\Lambda_0) = r$, and (1.8) implies that the column vectors of γ are elements of the orthogonal complement of Λ_0.

COROLLARY 1.7. *Let* $x \in \mathbb{R}^n$, *then* $x \in \Lambda_0$ *if and only if* $\gamma^T x = 0$.

EXAMPLE 1.8. For the chemical system in example 1.1 we have

$$(1.13) \qquad \Lambda_0 = \{\lambda \begin{pmatrix} 0 \\ 0 \\ 2 \\ -1 \end{pmatrix} + \mu \begin{pmatrix} 1 \\ 2 \\ -2 \\ 0 \end{pmatrix} \mid \lambda, \mu \in \mathbb{R}\}.$$

In this case $r = 2$, $n = 4$, $r(\beta) = r(\gamma) = 2$. As a consequence we can take $\gamma = \beta$.

In this chapter, we only consider *uniform systems*, i.e., systems having no space variations. A uniform system is specified by the values of the state variables at a single point of the reactor tank.

2. DIFFERENTIAL EQUATIONS OF CHEMICAL REACTIONS

In this and the following sections we consider two types of ordinary differential equations associated with homogeneous and uniform chemical systems. In each case the equations are formulated in terms of the *reaction rates* f_j, $j = 1,\dots,r$ of the r reactions in (1.1). These *rate functions* (or *rate laws* or *kinetics*) are functions of the state variables $c_1,\dots,c_n$. Also the vector functions $f(c)$ and $F(c)$,

$$(2.1) \qquad f = \begin{pmatrix} f_1 \\ \vdots \\ f_r \end{pmatrix}, \qquad F = \begin{pmatrix} F_1 \\ \vdots \\ F_n \end{pmatrix},$$

related by

$$(2.2) \qquad F = \nu^T f,$$

are used. F_i is the total production of M_i in moles per unit volume per unit time due to chemical reactions. Explicitly we have

$$(2.3) \qquad F_j(c) = \sum_{i=1}^{r} \nu_{ij} f_i(c), \qquad j = 1,\dots,n.$$

<u>REMARK 2.1</u>. A more realistic model is obtained by regarding the temperature T of the system as a state variable as well. In that case the functions f_j are given as functions of T. In this chapter, however, the temperature, and effects of its variations with time, will not be considered. The suppression of T from the formulas does not change the discussion in a relevant way. The reason for the simplification of the model is only based on the wish of considering a convenient mathematical model.

A *closed system* is a system (1.1) of constant volume which does not exchange mass or energy with its surroundings. It is convenient, to consider a closed system of unit volume. The time evolution of this system is described by the system of differential equations

$$(2.4) \qquad \frac{dc}{dt} = F(c), \qquad c(0) = c_0$$

We also consider in this chapter *open systems*, but the discussion will be limited to simple open systems known in chemical engineering as a *continuous stirred tank reactor*. Figure 1 shows such a system in which mass is exchanged with the surroundings.

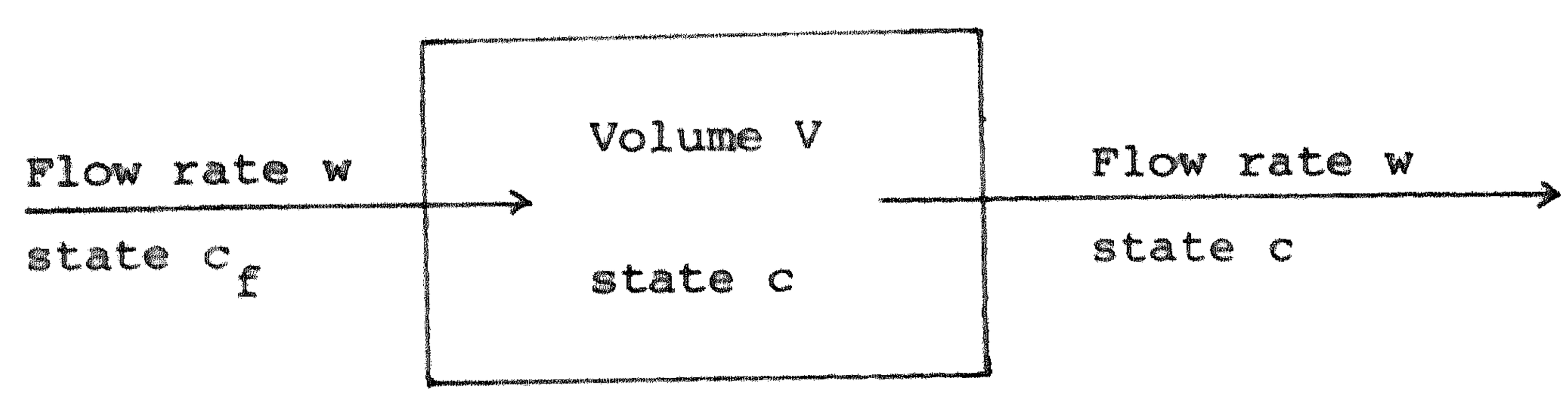

Figure 1

The volume V and the volumetric flow rate w of input and output streams are kept constant; $\theta = V/w$ is called the *holding time* of the reactor; c_f is the input or *feed state* variable and, as c, $c_f \in \mathbb{R}^n_+$. Its components are denoted by $c_{1f},\ldots,c_{nf}$, that is

$$(2.5) \qquad c_f = \begin{pmatrix} c_{1f} \\ \vdots \\ c_{nf} \end{pmatrix} .$$

The feed state may vary with time in which case we have a variable inflow.

The conservation equations for the chemical species can be written as

$$(2.6) \qquad \frac{dc}{dt} = \frac{1}{\theta}(c_f - c) + F(c), \qquad c(0) = c_0$$

For both closed and open systems we impose the following condition on the function F.

<u>POSTULATE 2.2.</u>

(i) The function $F\colon \mathbb{R}^n \to \mathbb{R}^n$ is continuous in $\mathbb{R}^n_+$.

(ii) For any $c_j = 0$, $\quad F_j \geq 0$.

<u>REMARK 2.3</u>. On account of condition (i) a conclusion may be drawn concerning the existence of solutions of (2.4) and (2.6). According to a result of Peano, the existence on some interval $[0,t_1)$ can be proved. See HALE [2] for a proof based on a fixed point theorem of Schauder, which is not proved by Hale. Gavalas, also using this fixed point theorem, gives a proof based on degree theory for completely continuous operators; this theory will be

given in chapter VI. A more elementary proof of the existence of solutions can be found in CODDINGTON & LEVINSON [3]. See also remark 3.4. As for uniqueness of the solutions, which is expected on physical grounds, the conditions of postulate 2.2 are not sufficient. If, however, F is Lipschitzian in $\mathbb{R}^n_+$ the initial value problem has at most one solution.

REMARK 2.4. On physical grounds, all state variables have to be non-negative, that is, c has to be an element of $\mathbb{R}^n_+$. Condition (ii) of the postulate insures the non-negativity of the state variables for all $t \geq 0$, if the initial value is chosen in $\mathbb{R}^n_+$.

REMARK 2.5. Condition (ii) of the postulate can be written as $(F,n) \geq 0$ on $\partial\mathbb{R}^n_+$, where n is the inward normal on the boundaries of $\mathbb{R}^n_+$.

In chemical experiments, often there are more than one equivalent systems of reactions (1.1) capable of describing a given chemical change, each system having its own rates f_j. The rates F_i, however, are the same for all equivalent systems. The descriptions in terms of f and F are both useful. The quantities that can be directly measured during the experiment are, among others, the pressure, temperature, concentrations and the thermal and electrical conductivity. From such measurements it is possible to determine the number of independent reactions, but no distinction can be made among equivalent systems of reactions. The determination of the rates f and F from experimental data is a task both difficult and of limited accuracy. Summarizing, the construction of a mathematical or chemical model of chemical reactions falls apart into the choice of (1.1) and into the choice of the rates f_j.

3. CLOSED SYSTEMS

We consider the differential equation (2.4) and we suppose that F satisfies the conditions of postulate 2.2. As noted in remark 2.4, a trajectory starting in $\mathbb{R}_+^n$ will remain in this region at all subsequent times. In the following subsection it will be shown that trajectories remain in a bounded r-dimensional region of $\mathbb{R}_+^n$.

3.1. INVARIANT MANIFOLDS

From (2.4), (1.8), (2.2) and $(\nu\gamma)^T = \gamma^T\nu^T$ we derive

$$\gamma^T \frac{dc}{dt} = \gamma^T F(c) = \gamma^T \nu^T f(c) = 0 \tag{3.1}$$

and integration gives

$$\gamma^T c(t) = \text{constant}.$$

The constant can be expressed in the initial value c_0 of c, giving

$$\gamma^T c(t) = \gamma^T c_0, \tag{3.2}$$

or

$$\gamma^T (c(t) - c_0) = 0. \tag{3.3}$$

Hence, as follows from corollary 1.7, any solution of (2.4) with initial value c_0 satisfies

$$c(t) - c_0 \in \Lambda_0, \tag{3.4}$$

or

$$c(t) \in \Lambda(c_0), \tag{3.5}$$

where $\Lambda(c_0)$ is the r-dimensional linear manifold

$$\Lambda(c_0) = \{x \in \mathbb{R}^n \mid x = c_0 + y,\ y \in \Lambda_0\}, \tag{3.6}$$

which can also be denoted by

$$\Lambda(c_0) = c_0 + \Lambda_0, \tag{3.7}$$

where in the notation the dependence on c_0 is emphasized.

The linear manifold $\Lambda(c_0)$ in $\mathbb{R}^n$ extends to values outside the positive orthant $\mathbb{R}^n_+$. Since we are only interested in values of the state variables in $\mathbb{R}^n_+$, it is convenient to consider only the intersection of $\Lambda(c_0)$ with $\mathbb{R}^n_+$.

<u>DEFINITION 3.1</u>. The set

$$\Lambda^+(c_0) = \mathbb{R}^n_+ \cap \Lambda(c_0) \tag{3.8}$$

is called the *invariant manifold corresponding to the point* c_0.

<u>REMARK 3.2</u>. The invariant manifold $\Lambda^+(c_0)$ is constructed without knowledge of the right-hand side of (2.4), that is, without the reaction rates f_j.

In terms of the elements of γ_{ij} of the matrix γ, the elements c of $\Lambda(c_0)$ satisfy the relations

$$\sum_{j=1}^{n} \gamma_{jk}\, c_j(t) = \sum_{j=1}^{n} \gamma_{jk}\, c_{j0}, \quad k = 1,\dots,n-r. \tag{3.9}$$

<u>LEMMA 3.3</u>. $\Lambda^+(c_0)$ *is closed, convex and bounded in* $\mathbb{R}^n_+$.

<u>PROOF</u>. The closedness follows from (1.12), (3.8) and (3.9). To show the convexity, let x and y be any two points of $\Lambda^+(c_0)$, then $c(s) = s\,x + (1-s)\,y \in \mathbb{R}^n_+$ and $\gamma^T c(s) = \gamma^T c_0$, $s \in [0,1]$. Hence $c(s) \in \Lambda^+(c_0)$. The boundedness follows from (1.9) and (3.9). Namely,

$$\sum_{k=1}^{r(\beta)} \sum_{j=1}^{n} \gamma_{jk}\, c_j(t) = \sum_{j=1}^{n} p_j\, c_j(t) = \sum_{j=1}^{n} p_j\, c_{j0}$$

and, since all p_j are positive, $c_j(t)$ must be bounded for all $t \geq 0$. □

Since a trajectory of equation (2.4) departing from c_0 lies entirely in $\Lambda^+(c_0)$, we can find c_{im}, $i = 1,\dots,n$ such that for any t

$$0 \le c_i(t) \le c_{im}, \qquad i = 1,\dots,n$$

or, if c_m is the vector with components c_{im},

$$(3.10) \qquad |c(t)| \le |c_m|.$$

The vector c_m is independent of the reaction rates f_j and is obtained without knowledge of the solution of (2.4). Hence $|c_m|$ is an a priori bound for $|c(t)|$ and this bound depends only on the initial condition.

REMARK 3.4. With this a priori bound we can verify that a solution is defined for all $t \ge 0$, and not only, as noted in remark 2.3, on some interval $[0,t_1]$. See HALE [2,pp. 17-18].

3.2 EXTENTS OF REACTIONS

As we have seen in the foregoing subsection, the action takes place in an r-dimensional linear manifold $\Lambda(c_0)$ of $\mathbb{R}^n_+$. In the subspace Λ_0 we can use intrinsic coordinates $\{\xi_1,\dots,\xi_r\}$ and, if $c \in \Lambda(c_0)$, c can be expressed in terms of c_0 and $\xi_1,\dots,\xi_r$. A convenient way of doing this is using the matrix ν. Since $r(\nu) = 4$, we can associate with ν a linear mapping, which induces an isomorphism between $\Lambda(c_0)$ and its image $\tilde{\Lambda}$, the r-dimensional ξ-space. Let us take, if $c-c_0 \in \Lambda_0$,

$$(3.11) \qquad c - c_0 = \nu^T\xi,$$

where

$$(3.12) \qquad \xi = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_r \end{pmatrix}$$

is an element of $\mathbb{R}^r$. The connection between the c and the ξ vector is as follows. Since $c-c_0 \in \Lambda_0$, it can be written as $c-c_0 = \lambda_1\nu_1 + \dots + \lambda_r\nu_r$, where ν_i are the row vectors of the matrix ν (see remark 1.6) and $\lambda_i \in \mathbb{R}$, $i = 1,\dots,r$. From (3.11) it follows that $\lambda_i = \xi_i$, $i = 1,\dots,r$.

REMARK 3.5. The variable ξ_j represents the contribution of the j-th reaction in the change from the state c_0 to the state c and is called the *extent of the j-th reaction*. The extents may be interpreted as degrees of freedom in the thermodynamic sense.

The image of $\Lambda^+(c_0)$ under the mapping (3.11) will be denoted by $\tilde{\Lambda}(c_0)$. From its construction it is clear, that $\tilde{\Lambda}(c_0)$ is a simplex in $\mathbb{R}^r$, that is a line segment if $r = 1$, a triangle (including the plane region with its bounds) if $r = 2$; a three-dimensional simplex is a tetrahedron. The simplex $\tilde{\Lambda}(c_0)$ contains the origin. The elements ξ of $\tilde{\Lambda}(c_0)$ satisfy, since $c \in \mathbb{R}^n_+$,

(3.13) $$c_{j0} + \sum_{i=1}^{n} \nu_{ij}\, \xi_i \geq 0, \qquad j = 1,\dots,n.$$

<u>EXAMPLE 3.6</u>. The extents for the reactions in example 1.1 with

$$c_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ c_{40} \end{pmatrix}$$

are given by

$$\begin{aligned} c_1 &= \xi_2, \\ c_2 &= 2\xi_2, \\ c_3 &= 2\xi_1 - 2\xi_2, \\ c_4 - c_{40} &= -\xi_1. \end{aligned}$$

These equations can be solved uniquely for ξ in terms of c, provided $c - c_0 \in \Lambda_0$, where Λ_0 is given in (1.13). The simplex $\tilde{\Lambda}(c_0)$ in this example is determined by the inequalities $c_i \geq 0$, giving

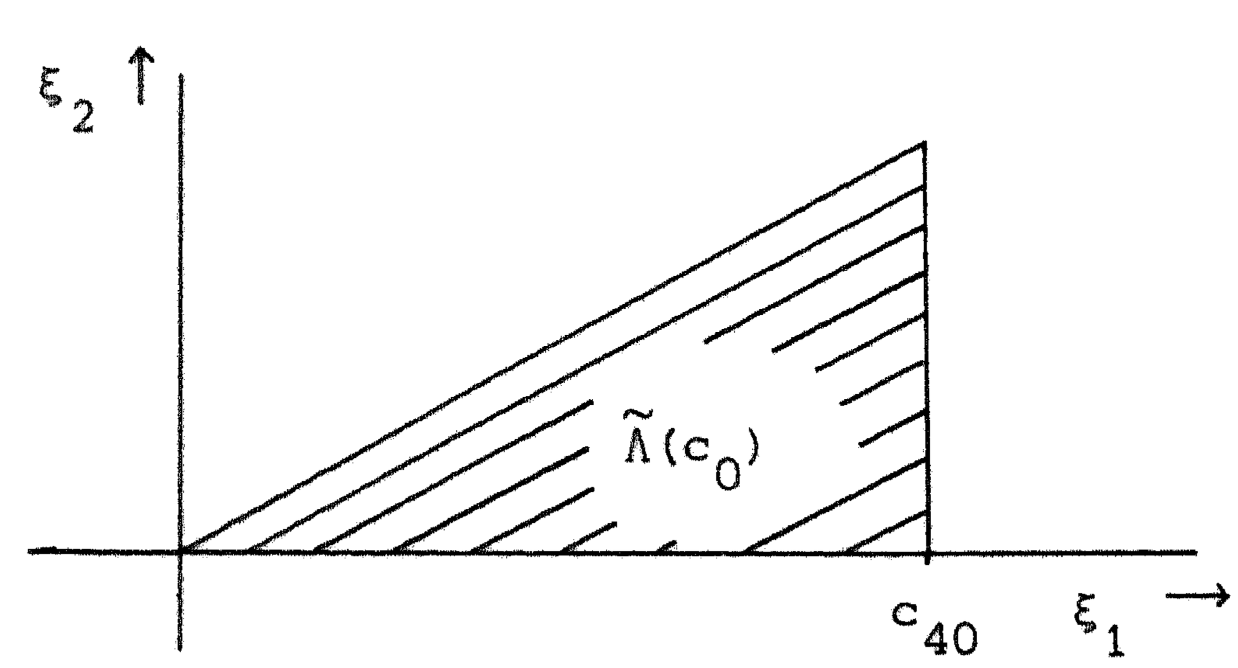

Figure 2

In terms of the extents ξ_j, the system (2.4) of equations reduces to a system of r equations (see 2.2) and (3.11))

$$(3.14) \qquad \frac{d\xi}{dt} = \tilde{f}(\xi), \; \xi(0) = 0,$$

where $\tilde{f}(\xi) = f(c)$, $c \in \Lambda^+(c_0)$ and $c = \nu^T\xi + c_0$. If $c \in \Lambda(c_0)$, (2.4) and (3.14) are equivalent.

REMARK 3.7. Condition (ii) of postulate 2.2 can be written as $(\tilde{f},n) \geq 0$ on $\partial\Lambda(c_0)$; see remark 2.5; n is the inward normal on $\partial\Lambda(c_0)$. The inner product and norm in $\mathbb{R}^r$ are as in $\mathbb{R}^n$.

3.3 EQUILIBRIUM POINTS

DEFINITION 3.8. A *kinetic equilibrium point* (or *equilibrium point* or *equilibrium state*) of a chemical system described by the differential equation (2.4) is a solution of the equation

$$(3.15) \qquad F(c) = 0.$$

LEMMA 3.9. *Let* f *and* F *be related by* (2.2). *Then* f *and* F *have the same zeros.*

PROOF. Suppose $f(c) = 0$, than trivially $F(c) = 0$. Conversely, suppose $F(c) = 0$, than $\nu^T f(c) = 0$, hence $f_1 \nu_1 + \ldots . f_r \nu_r = 0$, where $\{\nu_1, \ldots, \nu_r\}$ are the linearly independent row vectors of ν. Hence $f_i = 0$, $i = 1,\ldots,r$, and thus $f(c) = 0$. □

REMARK 3.10. Let c be an equilibrium state in $\Lambda(c_0)$, then $\tilde{f}(\xi) = 0$, where c and ξ are related by (3.11). Conversely, $\tilde{f}(\xi) = 0$ implies $f(c) = 0$. The corresponding point ξ will also be called an equilibrium point.

Of course, we are interested in equilibrium states in $\Lambda^+(c_0)$, or equivalently, in the simplex $\tilde{\Lambda}(c_0)$. In order to prove that equilibrium points exist, we calculate the degree of $\tilde{f}$ with respect to the simplex $\tilde{\Lambda}(c_0)$. The interior of the closed simplex will be denoted by $\tilde{\Lambda}^\circ(c_0)$; that is,

$$\tilde{\Lambda}^\circ(c_0) = \tilde{\Lambda}(c_0) - \partial\tilde{\Lambda}(c_0).$$

<u>THEOREM 3.11</u>. *A chemical system with differential equation* (2.4) *has at least one equilibrium point in* $\Lambda(c_0)$.

<u>PROOF</u>. We will prove that if $F \neq 0$ on $\partial\Lambda^+(c_0)$, or equivalently, $\tilde{f} \neq 0$ on $\partial\tilde{\Lambda}(c_0)$, $\tilde{f}$ has at least one zero in $\tilde{\Lambda}^\circ(c_0)$. Let us suppose $F \neq 0$ on $\partial\Lambda^+(c_0)$. The function $\tilde{f}$ is continuous and $\tilde{\Lambda}^\circ(c_0)$ is bounded. According to definition II.2.15, $\deg(\tilde{f},\tilde{\Lambda}^\circ(c_0),0)$ is defined, and we will prove that the degree is not zero. Let us consider the function $(\xi,t) \to h_t(\xi)$ given by

$$h_t(\xi) = (1-t)\,\tilde{f}(\xi) - t\,g(\xi) \tag{3.16}$$

where $g(\xi) = \xi - \xi^*$ and $\xi^* \in \tilde{\Lambda}^\circ(c_0)$; $h_t(\xi)$ is continuous on $\tilde{\Lambda}(c_0) \times [0,1]$ and, in order to apply theorem II.3.4, we verify if it has zeros in $\partial\tilde{\Lambda}(c_0) \times [0,1]$. The values $t = 0$, $t = 1$ are easily verified, since $h_0 = \tilde{f}$ and $h_1 = -g$ are supposed to be nonzero on $\partial\tilde{\Lambda}(c_0)$. Suppose now $h_t(\xi) = 0$ on $\partial\tilde{\Lambda}(c_0) \times (0,1)$. Then we obtain from (3.16)

$$\tilde{f}(\xi) = \frac{t}{1-t}\,(\xi-\xi^*).$$

Left side multiplication by ν^T yields

$$F(c) = \frac{t}{1-t}\,(c-c_0-c^* + c_0) = \frac{t}{1-t}\,(c-c^*),$$

where c^* is defined by $\nu^T\xi^* = c^* - c_0$; c^* is an interior point of $\mathbb{R}^n_+$ and $c \in \partial\,\mathbb{R}^n_+$. Some component of c, say c_k is zero, giving

$$F_k = \frac{t}{1-t}\,(-c_k^*).$$

But $c_k^* > 0$, and hence we have a contradiction with postulate 2.2. From theorem II.3.4 we obtain $\deg(h_t,\tilde{\Lambda}^\circ(c_0),0)$ = constant for $t \in [0,1]$ and hence $\deg(h_0,\tilde{\Lambda}^\circ(c_0),0) = \deg(h_1,\tilde{\Lambda}^\circ(c_0),0)$ giving

$$\deg(\tilde{f},\tilde{\Lambda}^\circ(c_0),0) = \deg(-g,\tilde{\Lambda}^\circ(c_0),0).$$

The right-hand side is easily computed using theorem II.3.5. The result is

$$\deg(\tilde{f},\tilde{\Lambda}^\circ(c_0),0) = (-1)^r. \tag{3.17}$$

An immediate consequence is, (see theorem II.3.2(b)) that equation (3.15) has at least one zero in $\Lambda^+(c_0)$. □

Figure 3 shows schematically the homotopic vector fields $\tilde{f}$ and $-g$, $g(\xi) = \xi-\xi^*$ with $\xi^* = 0$, for the case of two chemical reactions.

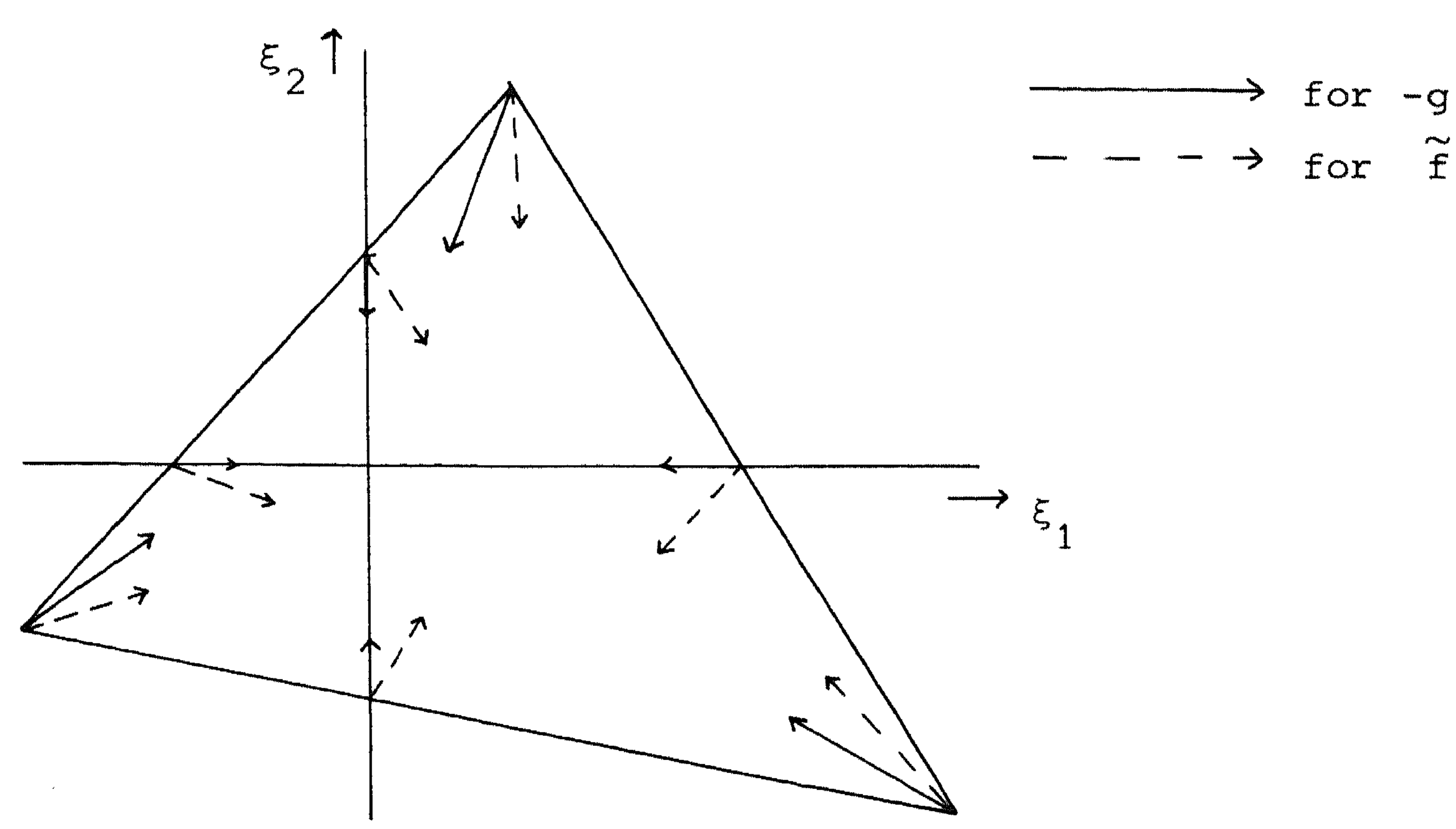

Figure 3

In the proof of theorem 3.11 $\deg(\tilde{f},\tilde{\Lambda}^\circ(c_0),0)$ is not computed if $\tilde{f}$ has zeros at $\partial\tilde{\Lambda}(c_0)$; in that case the degree is not defined. In order to obtain information about the zeros at $\partial\tilde{\Lambda}(c_0)$ we may attempt to compute the degree of $\tilde{f}$ with respect to a sufficiently large open ball B surrounding $\tilde{\Lambda}(c_0)$.

In calculating the degree of $\tilde{f}$ with respect to B, zeros of $\tilde{f}$ outside $\tilde{\Lambda}(c_0)$ must be considered as well. Such equilibrium points, however, do not have any physical significance, since all trajectories originating in $\tilde{\Lambda}(c_0)$ never leave this region, but these points do contribute to the degree of $\tilde{f}$. However, it is possible to extend the function $\tilde{f}$ outside $\tilde{\Lambda}(c_0)$ to a function $\tilde{\phi}$, such that

(i) $\tilde{\phi}(\xi) = f(\xi),\ \xi \in \tilde{\Lambda}(c_0)$,

(ii) $\tilde{\phi}$ is continuous in $\overline{B}$,

(iii) $\tilde{\phi} \neq 0$ outside $\tilde{\Lambda}(c_0)$.

The differential equation

$$(3.18)\qquad \frac{d\xi}{dt} = \tilde{\phi}(\xi),\ \xi(0) = 0$$

has the same solutions as (3.14) and the same equilibrium points in $\tilde{\Lambda}(c_0)$.

Before defining $\tilde{\phi}$, we introduce two auxiliary functions. The first one is the distance function d: $\mathbb{R}^r \to \mathbb{R}$ given by

$$d(\xi) = \inf\{|\xi-\xi^*| \mid \xi^* \in \tilde{\Lambda}(c_0)\},$$

the distance between ξ and the closed simplex $\tilde{\Lambda}(c_0)$. The second auxiliary function is p: $\mathbb{R}^r \to \mathbb{R}^r$, defined as the point of intersection of the line segment (ξ^*,ξ) with $\partial\tilde{\Lambda}(c_0)$, where $\xi^* \in \tilde{\Lambda}^\circ(c_0)$. In two dimensions the situation is as in figure 4.

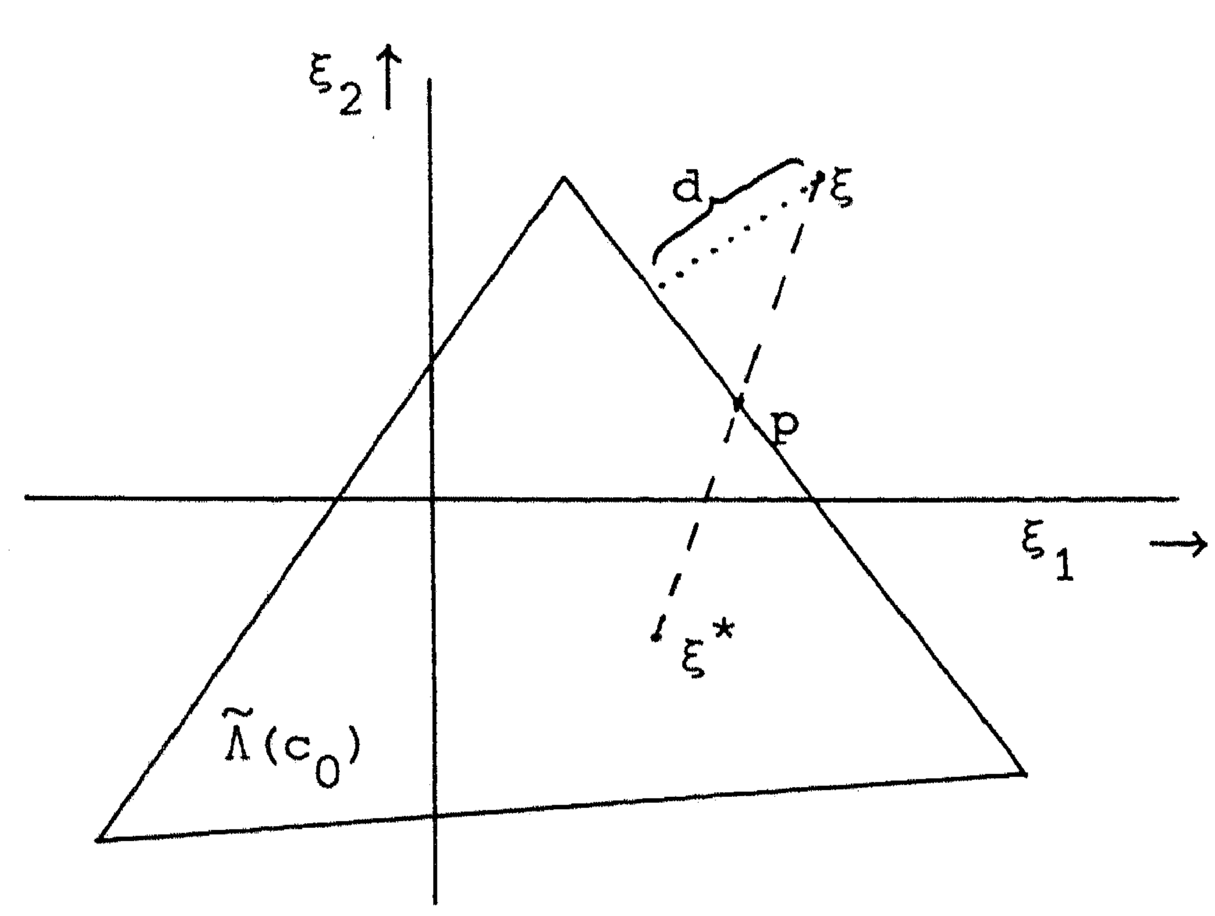

Figure 4

Let us now define $\tilde{\phi}$ as

$$(3.19)\qquad \tilde{\phi}(\xi) = \begin{cases} \tilde{f}(\xi), \text{ if } \xi \in \tilde{\Lambda}(c_0), \\ \tilde{f}(p(\xi)) - d(\xi)(\xi-\xi^*), \text{ if } \xi \notin \tilde{\Lambda}(c_0). \end{cases}$$

From its definition it is clear that $\tilde{\phi}$ is continuous if $\tilde{f}$ is continuous. Suppose $\tilde{\phi}(\xi) = 0$ outside $\tilde{\Lambda}(c_0)$. Then $\tilde{f}(p(\xi)) = d(\xi)(\xi-\xi^*)$, or by multiplying with ν^T, $F(p(c)) = d(\xi)(c-c^*)$, where $p(c)$ is the point in $\mathbb{R}^n$ corresponding to $p(\xi)$, and $c^*-c_0 = \nu^T\xi^*$. Since $p(\xi) \in \partial\tilde{\Lambda}(c_0)$, $p(c) \in \partial\mathbb{R}^n_+$; c^* is an interior point of $\Lambda(c_0)$. Moreover, since $\xi \notin \tilde{\Lambda}(c_0)$, $c \notin \mathbb{R}^n_+$, and hence, some component of c, say c_k, is negative, giving $F_k(p(c)) = d(c_k-c_k^*)$; since $c_k^* > 0$, $F_k(p(c)) < 0$, in contradiction with postulate 2.2. It follows that $\tilde{\phi}$ does not have any zeros outside $\tilde{\Lambda}(c_0)$. Hence $\deg(\tilde{\phi},B,0)$ is defined if $\tilde{\Lambda}(c_0)$ lies wholly in the ball B. As in the proof of theorem 3.11 we now can compute the degree which is left to the reader as an exercise. The result is given in the following theorem.

THEOREM 3.12. *Let* F *satisfy the conditions of postulate* 2.2, *let* $\tilde{\phi}$ *be an extension of* $\tilde{f}$ *as given in* (3.19), *and let* $\Omega \subset \mathbb{R}^r$ *be any open bounded set containing* $\tilde{\Lambda}(c_0)$, *then*

$$\deg(\tilde{\phi},\Omega,0) = (-1)^r.$$

The extension $\tilde{\phi}$ defined on the ξ-space $\mathbb{R}^r$ induces a function ϕ: $\Lambda(c_0) \to \mathbb{R}^r$ by writing $\phi(c) = \tilde{\phi}(\xi)$, where c and ξ are related by $c-c_0 = \nu^T\xi$, $c \in \Lambda(c_0)$. The function ϕ is an extension of f outside $\Lambda^+(c_0)$, such that $\phi(c) \neq 0$ outside $\Lambda^+(c_0)$. The function Φ: $\Lambda(c_0) \to \mathbb{R}^n$, given by $\Phi = \nu^T\phi$ is an extension of F. It should be noted that ϕ and Φ are defined only on $\Lambda(c_0)$.

REMARK 3.13. In general, the zeros of f are not isolated. To see this, we observe that f is a mapping $\mathbb{R}^n \to \mathbb{R}^r$ and $r < n$. Hence, generally, the equation $f(c) = 0$ defines a $(n-r)$-dimensional closed manifold $N(f) \subset \mathbb{R}^n$ of zeros of f. From theorem 3.11, it follows that $\Lambda^+(c_0)$ and $N(f)$ have at least one common point, whatever $c_0 \in \mathbb{R}^n$. Since c_0 may be arbitrarily close to 0, f is continuous and $N(f)$ is closed, 0 is an element of $N(f)$; that is, $f(0) = F(0) = 0$. Also $N(f)$ is unbounded.

3.4 THE NUMBER AND STABILITY OF EQUILIBRIUM POINTS

Theorem 3.11 gives the existence of at least one equilibrium point, but nothing is said about the exact number of such points. If we impose certain conditions on the rate functions f_j it is possible to prove that all trajectories in Λ^+ converge to a single equilibrium point. These conditions can be interpreted in a thermodynamical sense and are related to the consistency between thermodynamics and kinetics. The entropy function of the closed system plays the role of a Lyapunov function by which the convergence of the trajectories can be proved. For details, the reader is referred to GAVALAS [1, §1.5].

In the general case, when the reaction rates are only restricted by postulate 2.2, each invariant manifold may include more than one equilibrium point and it is interesting to obtain information about the number and stability of these points.

In order to give qualitative information, however, we need the differentiability of the rate functions. So, apart from the conditions in postulate 2.2, we demand that

$$\tilde{f} \in C(\tilde{\Lambda}(c_0)) \cap C^1(\tilde{\Lambda}^\circ(c_0)). \tag{3.20}$$

In the discussion of stability, the Jacobian matrix of a mapping, introduced in section II.2.1, plays an important role. For convenience, we give the following definition and notation for this matrix and its determinant.

DEFINITION 3.14. Let Ω be an open bounded set in $\mathbb{R}^n$; let $f \in C^1(\Omega)$. Then the linear operator $f'(x)\colon \mathbb{R}^n \to \mathbb{R}^n$, called *the derivative of f at x*, is given by the Jacobian matrix

$$f'(x) = \begin{pmatrix} \dfrac{\partial f_1(x)}{\partial x_1} & \cdots & \dfrac{\partial f_1(x)}{\partial x_n} \\ \vdots & & \vdots \\ \dfrac{\partial f_n(x)}{\partial x_1} & \cdots & \dfrac{\partial f_n(x)}{\partial x_n} \end{pmatrix} \tag{3.21}$$

and $J_f(x) = \det(f'(x))$ is the Jacobian determinant.

3.4.1 THE NUMBER OF EQUILIBRIUM POINTS

We know from theorem 3.12 and theorem II.3.14 that, for the case that $\tilde{f}(\xi) = 0$ has only a finite number of solutions,

$$\deg(\tilde{f},\Omega,0) = (-1)^r = \sum_{\xi\in\tilde{f}^{-1}(0)} \operatorname{ind}(\tilde{f},\xi,0), \tag{3.22}$$

where Ω is any open bounded set containing $\tilde{\Lambda}(c_0)$. Moreover, if $J_{\tilde{f}}(\xi^*) \neq 0$ at an isolated zero $\xi^* \in \tilde{\Lambda}^\circ(c_0)$, then as follows from theorem II.3.13

$$(3.23) \qquad \mathrm{ind}(\tilde{f},\xi^*,0) = (-1)^\sigma$$

where σ is the sum of the algebraic multiplicities of the real negative eigenvalues of $\tilde{f}'(\xi^*)$. Suppose now that all equilibrium points are in $\tilde{\Lambda}^\circ(c_0)$.

LEMMA 3.15. *If the number of equilibrium points in $\tilde{\Lambda}^\circ(c_0)$ is finite, and if $J_{\tilde{f}}(\xi) \neq 0$ at each equilibrium point, then the number of equilibrium points is odd, $2m+1$ say, among which $m+1$ have index $(-1)^r$ and the remaining m have index $(-1)^{r+1}$.*

PROOF. The index of each equilibrium point is +1 or -1, and the proof easily follows from (3.22). □

EXAMPLE 3.16. Consider a single reaction (r=1) in a closed system

$$M_1 - 2M_2 = 0.$$

The ν-matrix is (1 -2) and suppose that the system is described by the differential equation

$$\frac{dc}{dt} = F(c), \quad c(0) = c_0,$$

where $F(c) = \nu^T f(c) = \begin{pmatrix} f(c) \\ -2f(c) \end{pmatrix}$; $f\colon \mathbb{R}^2_+ \to \mathbb{R}$ is a given function such that F satisfies postulate 2.2. We introduce the extent ξ by writing $c-c_0 = \nu^T\xi$, hence

$$c_1 - c_{10} = \xi, \quad c_2 - c_{20} = -2\xi;$$

$\Lambda(c_0)$ is the line $2c_1 + c_2 = 2c_{10} + c_{20}$ and $\Lambda^+(c_0)$ is its intersection with $\mathbb{R}^2_+$. The simplex $\tilde{\Lambda}(c_0)$ is the segment $[-c_{10}, \frac{1}{2}c_{20}]$ on the ξ-axis and $\tilde{f}(\xi) = f(c_1,c_2) = f(\xi+c_{10}, -2\xi+c_{20})$. If $(F,n) \geq 0$ at $\partial\Lambda^+(c_0)$ (the points $(c_{10}+\frac{1}{2}c_{20},0)$ and $(0,2c_{10}+c_{20})$) then $\tilde{f}(-c_{10}) \geq 0$, $f(\frac{1}{2}c_{20}) \leq 0$. The following figures may be illustrative. Figure 5 gives the manifolds $\Lambda^+(c_0)$ and $\tilde{\Lambda}(c_0)$ in c-space and ξ-space. Figure 6 gives two possible functions $\tilde{f}$, which indeed are homotopic with $g(\xi) = -\xi$. Also the indices (+1) and (-1) of the equilibrium points are shown.

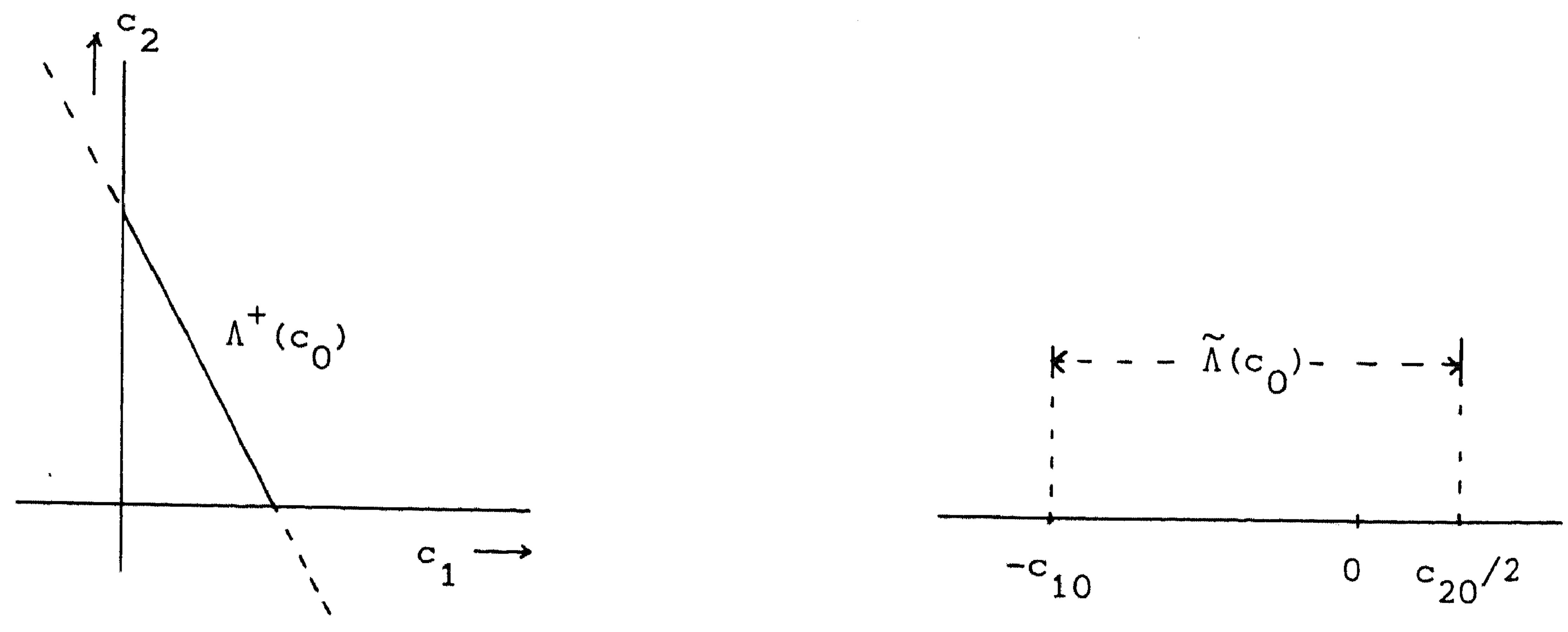

Figure 5

Figure 6

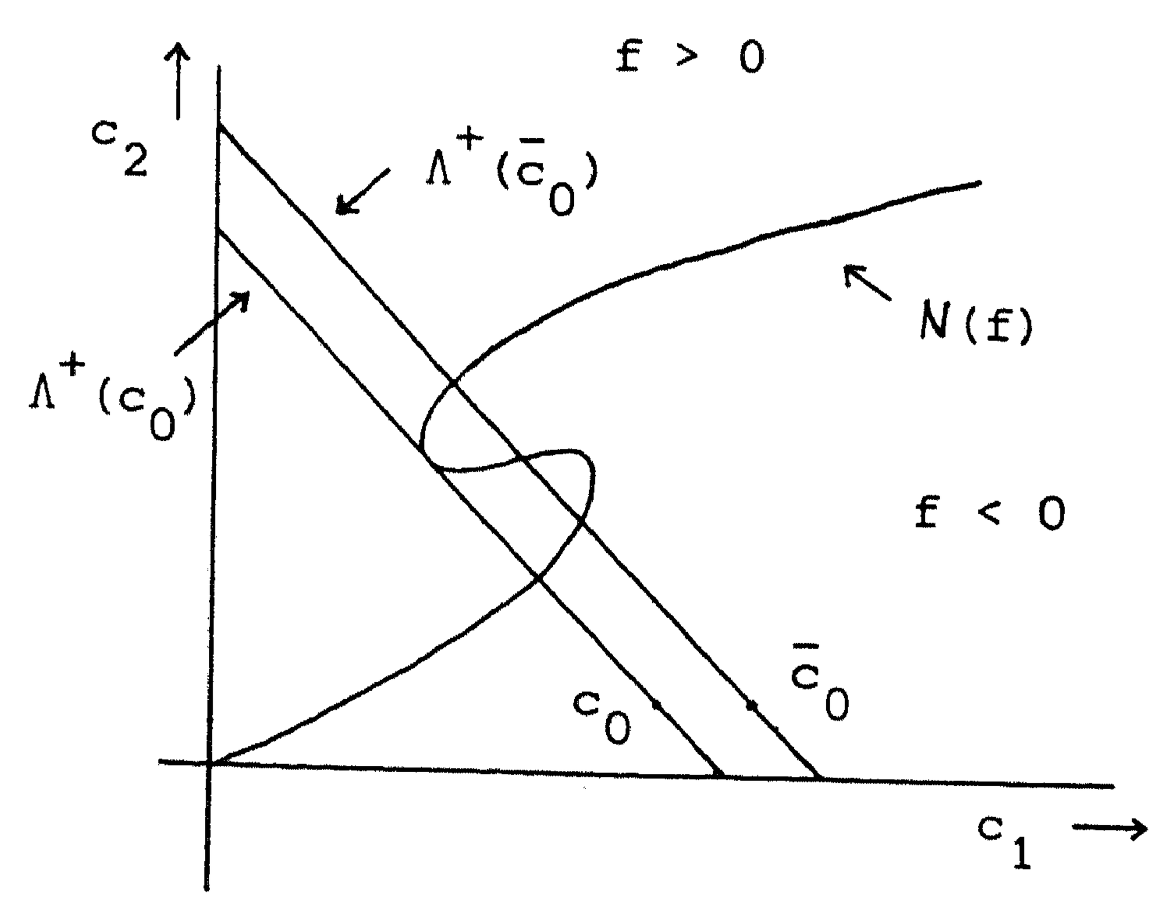

Figure 7

Figure 8

The vanishing of $J_{\tilde{f}}(\xi)$ at the equilibrium points may be illustrated by the set $N(f)$, introduced in remark 3.13. Figure 7 shows a situation where $J_{\tilde{f}}(\xi)$ will vanish at an equilibrium point in $\tilde{\Lambda}(c_0)$, while in $\tilde{\Lambda}(\bar{c}_0)$ this will not be the case.

The corresponding pictures in the ξ-space are shown in figure 8. It follows that, locally, the number of equilibrium points is 0, 1 or 2, according as the position of $\bar{c}_0$ with respect to $\Lambda(c_0)$. Generally, quite different situations may occur. In fact, in chapter IV an example will be given where the number of equilibrium points changes (locally) from 1 to 3.

3.4.2. THE STABILITY OF EQUILIBRIUM POINTS

We first give a definition of stability of an equilibrium point of a general differential equation

$$\begin{aligned} &\frac{dx}{dt} = F(x) \\ &x \in \mathbb{R}^n,\ F: \mathbb{R}^n \to \mathbb{R}^n, \end{aligned} \tag{3.24}$$

and we suppose that x^* is an equilibrium point, that is, $F(x^*) = 0$.

<u>DEFINITION 3.17</u>. The solution x^* is called *stable* if for any $\varepsilon > 0$ there exists a $\delta > 0$, such that any solution $x(t)$ of (3.24) with $x(0) = x_0$ satisfying $|x_0 - x^*| < \delta$, satisfies $|x(t) - x^*| < \varepsilon$, $t \geq 0$. The equilibrium point is said to be *asymptotically stable* if, in addition to being stable $|x(t) - x^*| \to 0$ as $t \to \infty$.

According to the Poincaré-Lyapunov theorem, the stability of an equilibrium point of (3.24) can be discussed by considering the eigenvalues of the Jacobian matrix $F'(x)$, defined in definition 3.14, at the equilibrium points. A sufficient condition for the stability (even asymptotic stability) of x^* is that all eigenvalues of $F'(x^*)$ have negative real parts. Conversely, if $F'(x^*)$ has one or more eigenvalues with positive real parts, the equilibrium point x^* is unstable. Finally, when $F'(x^*)$ has eigenvalues with zero real parts, no definitive statement about stability can be made without further information on $F(x)$.

Now suppose c^* is a kinetic equilibrium point of (2.4). This point defines a linear manifold $\Lambda(c^*)$, $c^* \in \Lambda(c^*)$. The image of $\Lambda^+(c^*)$ under the transformation of $c-c^* = \nu^T\xi$, with $c \in \Lambda^+(c^*)$, is a simplex $\tilde{\Lambda}(c^*)$ in the ξ-space. The point $\xi = 0$ corresponds to $c = c^*$; $\tilde{f}(0) = 0$, and hence $\xi = 0$ is an equilibrium point of (3.14). Suppose that the eigenvalues of $\tilde{f}'(0)$ have negative real parts. Then, according to Poincaré-Lyapunov, $\xi = 0$ is asymptotically stable. That is, given $\varepsilon > 0$, there exists a $\delta > 0$, such that $|\xi_0| < \delta$, $\xi_0 \in \tilde{\Lambda}(c^*)$, implies that a solution of (3.14), with $\xi(0) = \xi_0$ satisfies $|\xi(t)| < \varepsilon (t \geq 0)$ and moreover $\xi(t) \to 0$ as $t \to \infty$. The point ξ_0 corresponds to a point $c_0 \in \Lambda(c^*)$; c_0 is given by $c_0 - c^* = \nu^T\xi_0$. Hence, in $\Lambda(c^*)$, if $|c_0 - c^*|$ is small, then $c(t) \to c^*$, as $t \to \infty$, if $c(t)$ is a solution of (2.4) with $c(0) = c_0$.

The question arises: is c^* in the c-space asymptotically stable? The answer is negative. Take for instance an initial value $c_0 \notin \Lambda(c^*)$. Then the closed manifolds $\Lambda^+(c^*)$ and $\Lambda^+(c_0)$ have empty intersection. But $c(t) \in \Lambda^+(c_0)$ for all $t \geq 0$, and hence

$$(3.25) \qquad \lim_{t\to\infty} c(t) \neq c^*.$$

So, c^* is not asymptotically stable. (It is not possible to describe this situation in the ξ-space, since, if $c_0 \notin \Lambda^+(c^*)$, there is no corresponding initial value $\xi_0 \in \tilde{\Lambda}(c^*)$.)

From (3.25) it follows that $c(t)$ does not converge to c^*. But c^* is still stable, as will be proved in theorem 3.18.

Here arises another question. If c_0 is close to c^*, $c_0 \notin \Lambda(c^*)$, does the function $c(t)$ converge to a point $c_0^* \in \Lambda(c_0)$ close to c^* and is the corresponding point $\xi_0^* \in \tilde{\Lambda}(c_0)$, $c_0^* - c_0 = \nu^T\xi_0^*$, asymptotically stable? If the answer is affirmative, as indeed it is, then for the purpose of stability analysis there is no loss of generality in considering perturbations lying in the linear manifold of the equilibrium state, i.e., $c_0 \in \Lambda(c^*)$, or, equivalently, to discuss stability in the ξ-space.

<u>THEOREM 3.18</u>. *Let* $c^* \in \Lambda^+(c^*)$ *be an equilibrium point of* (2.4) *and let* $\xi = 0$ *be the corresponding equilibrium point of* (3.14), *where* $c-c^* = \nu^T\xi(c,c^*)$. *Let the real parts of the eigenvalues of* $\tilde{f}'(0)$ *be negative. Then the point* c^* *is a stable equilibrium point. Moreover it can be shown that if* $|c^*-c_0|$ *is small enough, then there exists a point* $c_0^* \in \Lambda^+(c_0)$, *such that* $c(t) \to c_0^*$, *where* $c(t)$ *is a solution of* (2.4) *with* $c(0) = c_0$, *and*

$|c^*-c_0^*| \to 0$. *The point* $\xi_0^* \in \tilde{\Lambda}(c_0)$, *where* c *and* ξ *are now related by* $c-c_0 = \nu^T\xi(c,c_0)$, $c \in \Lambda(c_0)$ *and* $c_0^*-c_0 = \nu^T\xi_0^*$, *is an asymptotically stable equilibrium point of* (3.14).

<u>PROOF</u>. Consider the equation $\tilde{f}(\xi(c,c^*)) = 0$. It has a solution $\xi = \xi(c^*,c^*) = 0$. The function $\tilde{f}$ can be considered as a function depending on ξ and on c^*. Let us make this clear by writing $\tilde{f}(\xi(c,c^*)) = \tilde{\phi}(\xi,c^*)$, where $\tilde{\phi}$: $\mathbb{R}^r \times \mathbb{R}^n \to \mathbb{R}^r$. The equation $\tilde{\phi}(\xi,c) = 0$ has a solution at $\xi = 0$, $c = c^*$. Moreover, the Jacobian matrix $\partial\tilde{\phi}(\xi,c)/\partial\xi$ of $\tilde{\phi}$ with respect to ξ satisfies $\det(\partial\tilde{\phi}(\xi,c^*)/\partial\varepsilon) \neq 0$ at $\xi = 0$. According to the implicit function theorem, for which the reader is referred to HALE [2,p.8], there exist neighbourhoods U and V of 0 and c^* in $\mathbb{R}^r$ and $\mathbb{R}^n$, respectively, such that for each fixed c in V the equation $\phi(\xi,c) = 0$ has a unique solution ξ in U. Furthermore, this solution can be given as $\xi = g(c)$, where g is continuous and $g(c^*) = 0$.

In $\mathbb{R}^n$ we choose an open ball $B_\delta(c^*) = \{c \in \mathbb{R}^n \mid |c-c^*| < \delta\}$. There exists a $\delta_1 > 0$ such that $\delta < \delta_1$ implies $B_\delta(c^*) \subset V$. Suppose now, $\delta < \delta_1$ and $c_0 \in B_\delta(c^*)$. There is a unique $\xi_0 = g(c_0)$ such that $\tilde{f}(\xi_0) = 0$. Since g is continuous and $g(c^*) = 0$, the smallness of $|c_0-c^*|$ implies the smallness of $|\xi_0|$, or, as needed in the future, that of $|\nu^T\xi_0|$. That is to say, given any $\varepsilon > 0$ we can find $\delta_2 > 0$ such that $\delta < \delta_2$ implies

(3.26) $$|\nu^T\xi_0| < \varepsilon/3.$$

Define $c_0^* \in \Lambda^+(c_0)$ as

(3.27) $$c_0^* = c_0 + \nu^T\xi_0,$$

giving an equilibrium point $c_0^* \in \Lambda^+(c_0)$ for (2.4).

Furthermore, we can find $\delta_3 > 0$ such that $\delta < \delta_3$ implies that for all $c \in B_\delta(c^*)$ the real parts of the eigenvalues of $\partial\tilde{\phi}(\xi,c)/\partial\xi$ evaluated at $\xi = g(c)$ are negative. This can be achieved since the eigenvalues depend continuously on c. Hence, if $\delta < \min(\delta_1,\delta_2,\delta_3)$, ξ_0 is asymptotically stable, and the point ξ_0^* mentioned in the theorem is ξ_0. Moreover, $|c^*-c_0^*| = |c^*-c_0 + c_0 - c_0^*| = |c^*-c_0 - \nu^T\xi_0| \to 0$ if $|c^*-c_0| \to 0$.

Let us now prove the stability of c^*. Since ξ_0 is asymptotically stable, we can find $\delta_4 > 0$ such that, for any initial value $\eta_0 \in \tilde{\Lambda}(c_0)$, $|\eta_0-\xi_0| < \delta_4$

implies $\xi(t) \to \xi_0$, where $\xi(t)$ is a solution of (3.14) with $\xi(0) = \eta_0$. So, with $\varepsilon > 0$ introduced earlier, we can choose δ_4 such that $|\eta_0-\xi_0| < \delta_4$ implies

$$(3.28) \qquad |\nu^T(\xi(t) - \xi_0)| < \varepsilon/3.$$

Define $\Gamma = \{c \in \Lambda^+(c_0) \mid c = c_0 + \nu^T\xi, |\xi-\xi_0| < \delta_4\}$.
Any solution with initial value $c_0 \in \Gamma$ satisfies $c(t) \to c_0^*$ as $t \to \infty$. Take $c_0 \in \Gamma \cap B_\delta(c^*)$ with $\delta < \min(\delta_1,\delta_2,\delta_3,\delta_4,\varepsilon/3)$. Observe that $|c(t) - c^*| = |c(t) - c_0^* + c_0^* - c_0 + c_0 - c^*| \le |c(t) - c_0^*| + |c_0^*-c_0| + |c_0-c^*|$. By using (3.26), (3.28), $c(t) - c_0^* = \nu^T(\xi-\xi_0)$ and $c_0^*-c_0 = \nu^T\xi_0$, we obtain $|c(t) - c^*| < \varepsilon$, $t \ge 0$, which proves the stability of c^*. □

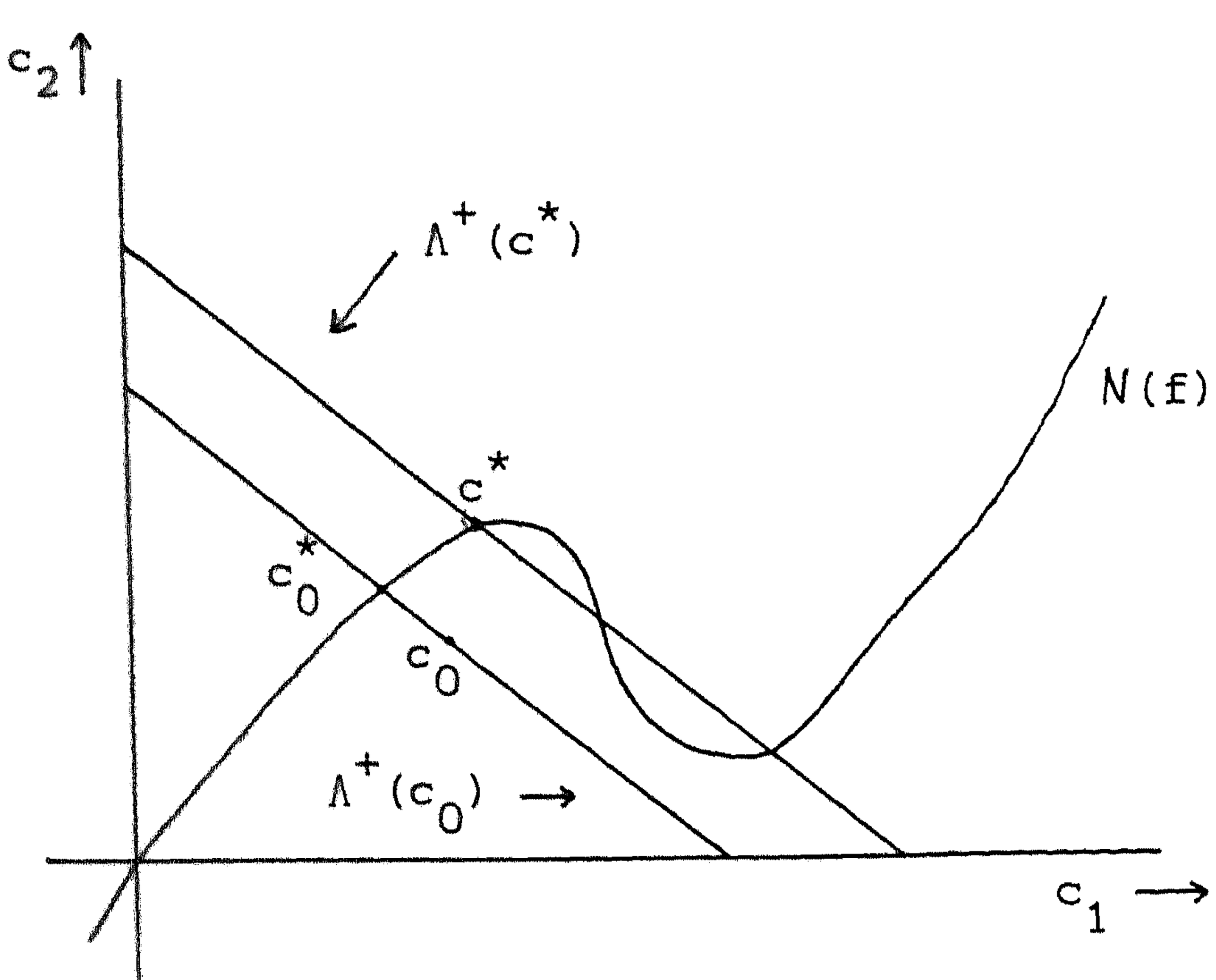

Figure 9

In figure 9 the situation is described for the case of one chemical reaction.

To obtain the relationship between the index and the stability in $\tilde{\Lambda}(c_0)$ of an equilibrium point ξ^* of the system (3.14), let us consider first an odd number r of chemical reactions. Then $\tilde{f}'(\xi^*)$ has an odd number of real eigenvalues. An index +1 implies, according to lemma 3.15, an even number of eigenvalues in $(-\infty,0)$ and hence an odd number of eigenvalues in $(0,\infty)$, so that the equilibrium state ξ^* is unstable. An index -1 implies an even number of positive eigenvalues. If $r = 1$, ξ^* is stable but if $r = 3,5,\ldots$ no conclusion about stability can be made. In any case, if the number of equilibrium points is $2m+1$, at least m of them are unstable.

When r is even, $\tilde{f}'(\xi^*)$ has an even number of eigenvalues. An index -1 implies an odd number of eigenvalues in $(-\infty,0)$ and an odd number in $(0,\infty)$, hence the equilibrium state ξ^* is unstable. An index $+1$ does not allow a conclusion about stability. Again, at least m among the $2m+1$ states are unstable. We have proved the following theorem

<u>THEOREM 3.19</u>. *An equilibrium state of* (3.14) *such that* $J_{\tilde{f}}(\xi^*) \neq 0$, *is unstable if its index satisfies* $\mathrm{ind}(\tilde{f},\xi^*,0)\times(-1)^r < 0$. *If* $J_{\tilde{f}}(\xi^*) \neq 0$ *for all the equilibrium states of a given manifold* $\tilde{\Lambda}$, *the number of these points is odd,* $2m+1$, *among which* m *at least are unstable.*

<u>COROLLARY 3.20</u>. *In the case of one chemical reaction,* $r = 1$, *m of the states are unstable and the remaining* $m+1$ *are stable. Thus for* $r = 1$, $m = 0$ *the unique equilibrium point is always stable. In figure* 6 *the cases* $r = 1$, $m = 0$ *and* $r = 1$, $m = 1$ *are drawn, respectively. An equilibrium point with index* -1 *is stable.*

4. OPEN SYSTEMS

As in section 3 we can use the matrix γ and we obtain in this case from (2.6)

$$(4.1) \qquad \begin{cases} \frac{da}{dt} + \frac{1}{\theta} a = \frac{1}{\theta} a_f \\ a(0) = a_0, \end{cases}$$

where $a = \gamma^T c$, $a_f = \gamma^T c_f$, $a_0 = \gamma^T c_0$ and the a-vectors are elements of $\mathbb{R}^{n-r}$.

Equation (4.1) gives on integration

$$(4.2) \qquad a(t) = e^{-t/\theta} a_0 + \theta^{-1} \int_0^t e^{-(t-\tau)/\theta} a_f(\tau) d\tau.$$

Hence we now have

$$(4.3) \qquad \gamma^T c(t) = a(t),$$

defining an integral manifold depending on t in contrast with closed systems, where the corresponding right-hand side of (4.3), see (3.2), is a constant. Again (4.3) defines a linear manifold $\Lambda^+(c_0, c_f, t)$. Considering bounded inputs $|a_f(t)| \le a_M$, $t \ge 0$, we obtain

$$|a| \le |a_0| + a_M.$$

Hence $|\gamma^T c(t)|$ is bounded and using the same argumentation as in section 3 we can prove that $\Lambda^+(c_0, c_f, t)$ is bounded for all t. From this it follows that the concentrations are subjected to a priori bounds and hence, if F in (2.6) satisfies the conditions of postulate 2.2, the existence of solutions can be proved.

4.1. STEADY STATES

From now on we suppose that the feed state c_f is a constant, which implies that (4.2) becomes

$$a(t) = e^{-t/\theta} a_0 + (1-e^{-t/\theta})\, a_f,$$

or

$$\gamma^T c(t) = \gamma^T\{e^{-t/\theta}c_0 + (1-e^{-t/\theta})c_f\}. \tag{4.4}$$

Hence the effect of the initial condition c_0 quickly disappears and the state of the system is eventually determined by the input variables c_f alone. More precisely, as $t \to \infty$ the state trajectories rapidly approach the r-dimensional linear manifold $\Lambda^+(c_f)$. These trajectories lie outside $\Lambda^+(c_0)$, except when $a_0 = a_f$, or $\gamma^T c_0 = \gamma^T c_f$, that is, when $c_0 \in \Lambda^+(c_f)$.

DEFINITION 4.1. A *steady state* is the solution of the time independent equation

$$c - c_f = \theta F(c). \tag{4.5}$$

In the ξ-space the steady states follow from

$$\xi = \theta\tilde{f}(\xi), \tag{4.6}$$

where the extents ξ are defined by (cf. 3.11)

$$c - c_f = \nu^T\xi, \qquad c \in \Lambda(c_f). \tag{4.7}$$

THEOREM 4.2. *If* F *satisfies the conditions of postulate* 2.2, *then the chemical system with differential equation* (2.6) *has one or more steady states in* $\Lambda^+(c_f)$.

PROOF. Let us write

$$g(\xi) = \xi - \theta\tilde{f}(\xi), \qquad h(\xi) = \xi - \xi_0, \tag{4.8}$$

where $\xi_0 \in \tilde{\Lambda}^\circ(c_f)$, and consider the mapping $(\xi,t) \to H_t(\xi)$ given by

$$H_t(\xi) = tg(\xi) + (1-t)h(\xi).$$

Proceeding as in theorem 3.11 we obtain, if $g \neq 0$ on $\partial\tilde{\Lambda}(c_f)$,

$$\deg(g,\tilde{\Lambda}^\circ(c_f),0) = \deg(h,\tilde{\Lambda}^\circ(c_f),0) = 1.$$

This proves the theorem. □

REMARK 4.3. As in section 3, we can extend the function $\tilde{f}$, or g, in such a way that the extension does not vanish outside $\tilde{\Lambda}(c_f)$. For any open bounded set $\Omega \supset \tilde{\Lambda}(c_f)$ we have $\deg(g,\Omega,0) = 1$, where g and its extension are denoted by the same symbol.

4.2. UNIQUENESS AND STABILITY OF STEADY STATES

The following lemma is the analogue of lemma 3.15; g is given by (4.8).

LEMMA 4.4. *If the number of steady states in* $\tilde{\Lambda}^{\circ}(c_f)$ *is finite, and if* $J_g(\xi_s) \neq 0$ *for all steady states* $\xi_s \in \tilde{\Lambda}^{\circ}(c_f)$ *and* $g \neq 0$ on $\partial\tilde{\Lambda}(c_f)$ *then the number of the steady states is odd,* $2m + 1$ *say, with* m *having index* -1 *and* $m + 1$ *having index* $+1$. *The index of the steady state* ξ_s *is equal to* $(-1)^{\sigma}$, *where* σ *is the sum of the algebraic multiplicities of the real eigenvalues of* $f'(\xi_s)$ *in the interval* $(1/\theta,\infty)$.

PROOF. Remark that the eigenvalues of $f'(\xi)$, say λ_i, and the eigenvalues of $\frac{1}{\theta} I_r - \tilde{f}'(\xi)$, say μ_i, satisfy $\mu_i = \lambda_i - \frac{1}{\theta}$. □

If θ is small, it may be expected that for each steady state ξ_s none of the real eigenvalues of $\tilde{f}'(\xi)$ are situated in $(1/\theta,\infty)$. In that case, the index of each point ξ_s, that is, $\mathrm{ind}(\mathrm{id}-\theta\tilde{f},\xi_s,0)$, is +1 from which follows that we have only one steady state. In order to prove this, we construct an upper bound for the real eigenvalues of $\tilde{f}'(\xi)$ which does not depend on σ. It is supposed that $\tilde{f} \in C^1(\tilde{\Lambda}(c_f))$.

First we introduce the real functional $B\colon \tilde{\Lambda}(c_f) \times \mathbb{R}^r \to \mathbb{R}$, defined by

$$(4.9) \qquad B(\xi,\rho) = \rho^T \tilde{f}'(\xi)\rho$$

where $\xi \in \tilde{\Lambda}(c_f)$ and $\rho \in \mathbb{R}^r$. B can be written as

$$B(\xi,\rho) = \sum_{i,j=1}^{r} \frac{\partial\tilde{f}_i(\xi)}{\partial\xi_j}\rho_i\rho_j, \qquad \rho = \begin{pmatrix}\rho_1\\ \vdots \\ \rho_r\end{pmatrix}.$$

Furthermore we write

$$(4.10) \qquad b(\xi) = \max_{|\rho|=1} B(\xi,\rho), \qquad b_m = \max_{\xi\in\tilde{\Lambda}(c_f)} b(\xi).$$

Suppose λ is a real eigenvalue of $\tilde{f}'(\xi_s)$ for some steady state ξ_s, and ρ_λ the corresponding eigenvector normed as $|\rho_\lambda| = 1$. Then

$$\lambda = B(\xi_s,\rho_\lambda) \le b(\xi_s) \le b_m.$$

Hence, if $\theta b_m < 1$, then $\lambda < 1/\theta$, giving an explicit bound of θ such that all real eigenvalues of $\tilde{f}'(\xi)$ are outside $(1/\theta,\infty)$. As a consequence, the index of any steady state is +1 if $\theta b_m < 1$. So we have proved the following theorem.

THEOREM 4.5. *Let* b_m *be defined as in* (4.9) *and* (4.10). *If* $\theta b_m < 1$, *then there is one and only one steady state* $\xi_s \in \tilde{\Lambda}(c_f)$.

For large θ we can also give information on the uniqueness of a steady state. Let us recall that an equilibrium point is a solution of $\tilde{f}(\xi) = 0$ and a steady state is a solution of (4.6) and depends on θ and c_f. The vector c_f defines a linear manifold $\Lambda(c_f) \subset \mathbb{R}^n$ and, if c and ξ are related by (4.7), each simplex $\tilde{\Lambda}(c_f)$ contains at least one equilibrium point (theorem 3.11) and at least one steady state (theorem 4.2). With these preliminaries we are ready to prove the following theorem.

THEOREM 4.6. *Let* $\xi_0 \in \tilde{\Lambda}(c_f)$ *be a unique equilibrium point and suppose that the eigenvalues of* $\tilde{f}'(\xi_0)$ *have negative real parts. Then there exists* $\theta^* > 0$, *such that* $\theta > \theta^*$ *implies that* $\tilde{\Lambda}(c_f)$ *contains a unique steady state* ξ_s *and the eigenvalues of* $\tilde{f}'(\xi_s)$ *have negative real parts.*

PROOF. If we set

$$\xi_m = \max_{\xi\in\tilde{\Lambda}(c_f)} |\xi|$$

then

$$|\tilde{f}(\xi_s)| \le \xi_m/\theta$$

for any solution $\xi_s \in \tilde{\Lambda}(c_f)$ of (4.6). But $\tilde{f}(\xi_0) = 0$, and ξ_0 is the only equilibrium point in the closed manifold $\tilde{\Lambda}(c_f)$. So, $|\xi_s-\xi_0|$ is small if θ is large. That is, for any $\varepsilon > 0$, there exists θ^* such that $\theta > \theta^*$ implies $|\xi_s-\xi_0| < \varepsilon$. But if ε is small enough, the eigenvalues of $\tilde{f}'(\xi_s)$

have negative real parts. In that case, $\mathrm{ind}(g,\xi_s,0) = 1$, and hence ξ_s is unique. $\square$

In open systems it is natural to consider perturbations in the initial state and the feed state, which suggests the following definition of stability.

<u>DEFINITION 4.7</u>. A steady state $c_s \in \Lambda(c_f)$ will be called stable if given any $\varepsilon > 0$ there exists a $\delta > 0$ such that $|c_0-c_s| < \delta$, $|c_f'-c_f| < \delta$ imply that the solution $c(t)$ of the equation

$$\text{(4.11)} \qquad \frac{dc}{dt} = \frac{1}{\theta}(c_f'-c) + F(c), \qquad c(0) = c_0$$

satisfies $|c(t)-c_s| < \varepsilon, \quad t \geq 0.$

In fugure 10 the situation is illustrated for one chemical reaction (r=1). Since the solution is attracted by $\Lambda(c_f')$, if $c_f' \notin \Lambda(c_f)$ the solution will never reach the point c_s.

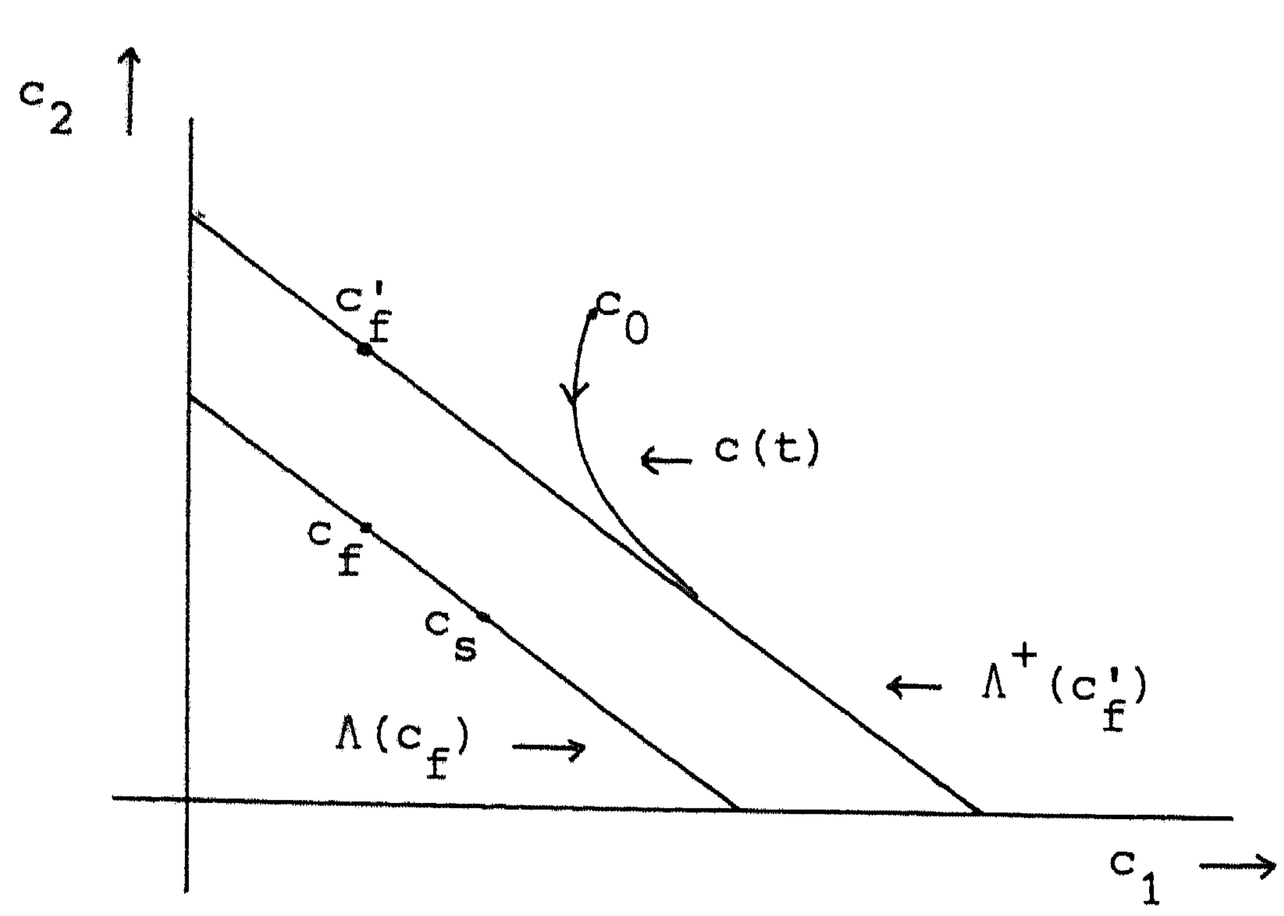

Figure 10

Under the condition of theorems 4.5 and 4.6, for small θ and for large θ, the steady state is unique. As in theorem 3.18 it can be proved that in these cases c_f is stable. Multiple steady states and instabilities are possible when the flow rate (corresponding to c_f) and the reaction rate (corresponding to F) balance each other. If either of the two rates predominates the steady state is unique and stable.

As in the previous section it can be shown that the stability of the steady state $c_s \in \Lambda(c_f)$ (under the perturbations c_0, c_f') is equivalent to the stability of the steady state $c_s' \in \Lambda(c_f')$ under the perturbation c_0, which again is equivalent to the asymptotic stability of c_s' under perturbation $c_0 \in \Lambda(c_f'))$.

REMARK 4.8. It should be emphasized that, if $c_0 \in \Lambda^+(c_f')$, corresponding to c_0 there is no point in $\tilde{\Lambda}(c_f)$ under the transformation $c - c_f' = \nu^T\xi$, $c \in \Lambda(c_f')$. Therefore, it is not possible to give a differential equation in terms of ξ in the simples $\tilde{\Lambda}(c_f')$ analogous with (3.14).

Using lemma 4.4 and the Poincaré-Lyapunov theorem we can prove the following theorem, the analogue of theorem 3.19.

THEOREM 4.9. *Under the conditions of lemma* 4.4, *at least* m *of the* 2m + 1 *steady states of a given manifold are unstable.*

EXAMPLE 4.10. Consider example 3.16. The simplex $\Lambda(c_f)$ is obtained by replacing c_0 by c_f. The steady state equation is $\xi = \theta\tilde{f}(\xi)$. An appropriate choice of f(c) gives the following picture.

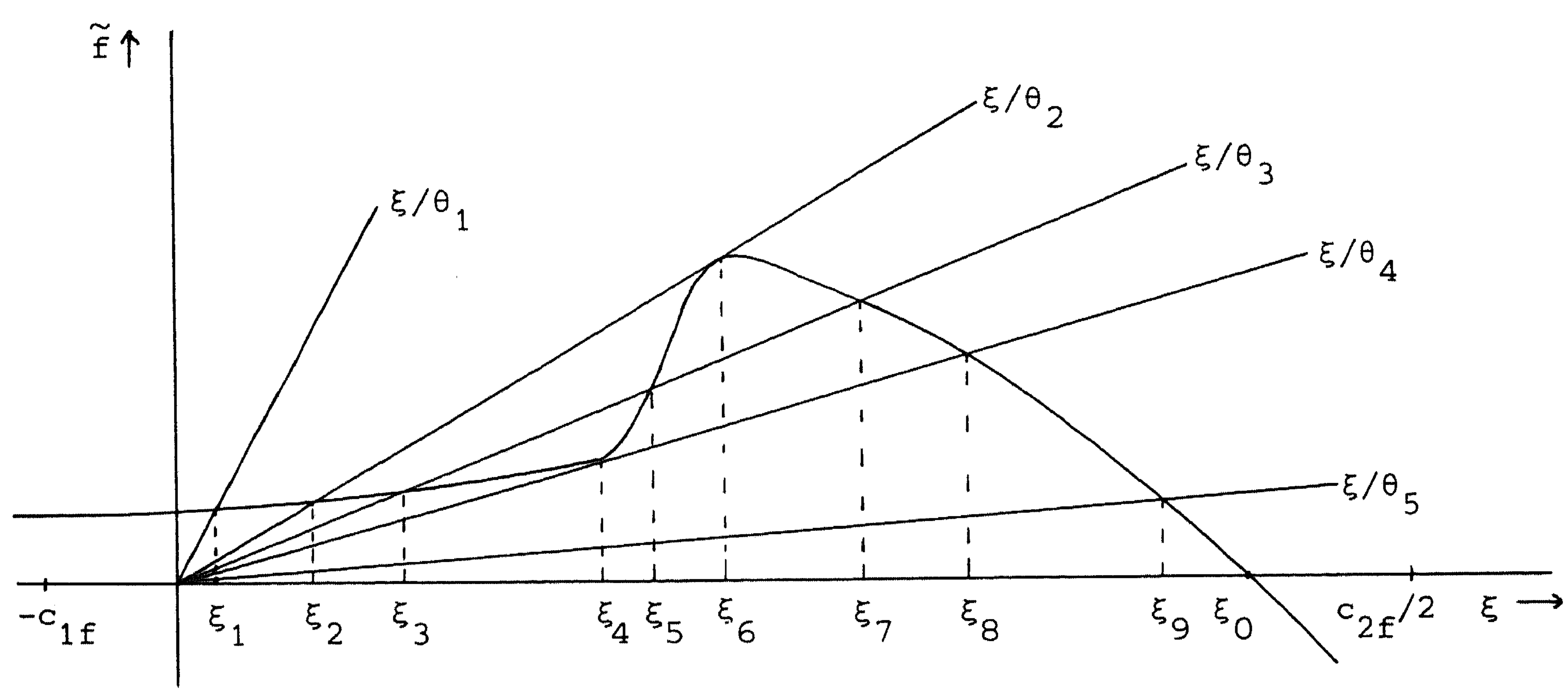

Figure 11

When θ is smaller than θ_2 or larger than θ_4 the steady state (e.g. ξ_1, ξ_9) is unique and stable. When $\theta = \theta_4$, or $\theta = \theta_2$, $d\tilde{f}/d\xi = 1/\theta$ and the index of the points ξ_4, ξ_6 is zero. For values of θ between θ_2, θ_4 there are three steady states. Steady states, such as ξ_5 have index -1, as $d\tilde{f}/d\xi > 1/\theta$, and are unstable. Steady states such as ξ_3 and ξ_9 have index +1, as $d\tilde{f}/d\xi < 1/\theta$, and are stable.

Figure 12 shows the curve of steady states in the ξ - θ plane. From this curve the regions of stability and instability are easily determined. A point on the curve is stable if $d\xi/d\theta > 0$.

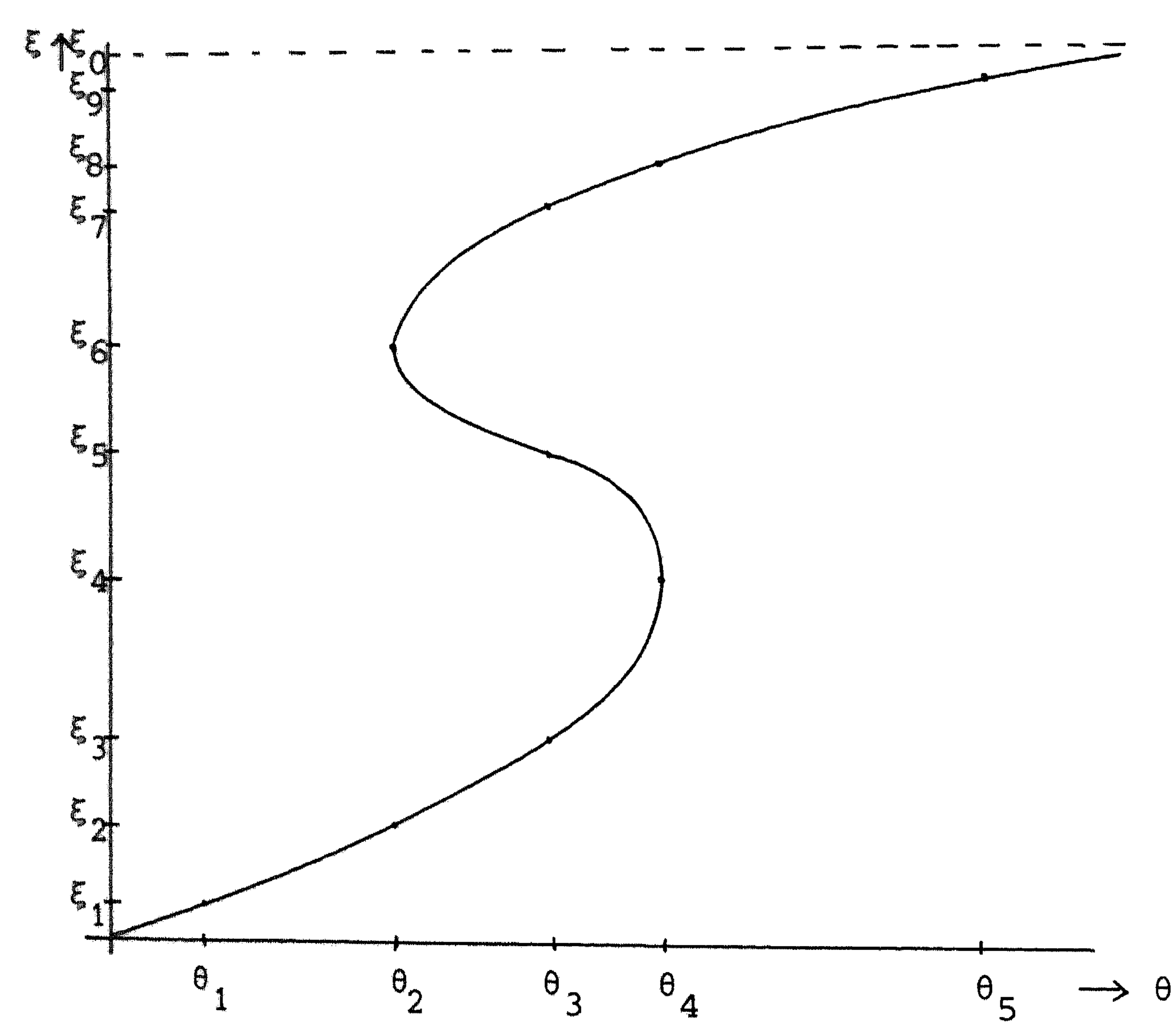

Figure 12

LITERATURE

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IV. BIFURCATION AND STABILITY OF STEADY STATES

1. INTRODUCTION

In the present chapter we will be concerned with some special features of equations

$$(1.1) \qquad F(x,\lambda) = 0,$$

where $F: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is a continuous differentiable mapping. The problem of finding solutions of (1.1) is called a *nonlinear eigenvalue problem*. However, the reader should interpret this term with some care. In most applications the function F depends nonlinearly on the variable x, but linearly on the parameter λ.

The distinction between x and λ is made because of the interpretation of $F(x,\lambda)$ as the right-hand side of an autonomous differential equation for x:

$$(1.2) \qquad \frac{dx}{dt} = F(x,\lambda).$$

The independent variable t will be called time, since this is the terminology encountered in most applications. Then x is the vector of state variables of the system, whereas λ is a parameter describing the physical configuration in which the evolution of the system takes place. Although in a concrete situation the value of λ may be known, we will study (1.1) and (1.2) without any specification of λ in advance. As a matter of fact our interest is primarily in changes of the qualitative behaviour of solutions of (1.2) with variations in λ.

For a given value of λ, the time independent solutions of (1.2) are precisely the points x such that (x,λ) is a solution of (1.1). Time independent solutions will be called *steady states* and the usual definition of stability (cf. definition III.3.17) is appropriate.

Already it has been remarked in the first chapter that the number of solutions of (1.1) may vary as λ varies. Bifurcation analysis is concerned with such variations, though under the restriction that only solutions in a small neighbourhood of a known solution are studied.

The solution set of (1.1) can be analysed without any reference to the differential equation (1.2), and in fact in sections 2, 3 and 4 no differential equation will occur. The interpretation of $F(x,\lambda)$ as the right-hand side of (1.2) only enters in the concept of stability. Discussion of stability of bifurcating solutions is postponed to section 5. There it will be shown that bifurcation usually is accompanied by changes in the stability character of the known solution, and thus by changes in the qualitative behaviour of solutions of (1.2). As examples we will treat some uniform open chemically reacting systems. In chapter III it was shown that such a system can be described by a differential equation

(1.3) $$\frac{dx}{dt} = -\frac{1}{\theta}x + f(x).$$

By choosing $\lambda = \frac{1}{\theta}$ we obtain an equation of the form (1.2), where indeed $F(x,\lambda) = f(x) - \lambda x$ is linear in λ.

In this chapter the main tools will be the degree of a mapping (especially the index or local degree) and the implicit function theorem. Our results will be of a qualitative nature, but we will also spend some time on the (local) construction of solutions in the neighbourhood of a known solution.

Although we limit ourselves explicitly to finite-dimensional nonlinear eigenvalue problems, part of our motivation lies in the introduction of concepts, ideas and methods of proof which will be generalized to mappings defined on Banach spaces in a later chapter. It is hoped that by the restriction to the finite-dimensional case the technical difficulties are minimized and that some of the underlying basic ideas are more easily demonstrated.

Most of the literature on bifurcation theory deals with mappings defined on Banach spaces and finite-dimensional problems are only used as illustrations. Nevertheless we emphasize that for the preparation of this chapter we have frequently made use of STAKGOLD [1], SATTINGER [2], KRASNOSEL'SKII [3], and FRAENKEL [4]. Finally we mention that most of the examples in section 3 are taken from STAKGOLD [1] and PIMBLEY [5].

2. FORMULATION OF THE BASIC PROBLEM AND SOME PRELIMINARY RESULTS

Let $F: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ be a continuous mapping. We shall consider the equation

$$(2.1) \qquad F(x,\lambda) = 0.$$

A *solution* of (2.1) is a pair (x,λ) such that equation (2.1) is satisfied. The *solution set* $F^{-1}(0)$ is defined by

$$F^{-1}(0) = \{(x,\lambda) \mid F(x,\lambda) = 0\}.$$

Now suppose there is an explicitly known simple curve

$$\Gamma = \{(x(\lambda),\lambda) \mid a \le \lambda \le b\}$$

that belongs to $F^{-1}(0)$. The known curve Γ will be called the *basic solution.*

DEFINITION 2.1. A point $\lambda_0 \in (a,b)$ is called a *bifurcation point* of (2.1) with respect to Γ if in every neighbourhood of $(x(\lambda_0),\lambda_0)$ there exists a solution (x,λ) not lying on Γ.

REMARK 2.2. Instead of bifurcation point the term *branch-point* is sometimes used.

REMARK 2.3. Note that the definition emphasizes small neighbourhoods of $(x(\lambda_0),\lambda_0)$.

Now the basic problem of bifurcation theory can be formulated as that of finding the bifurcation points of (2.1) and studying the structure of $F^{-1}(0)$ near such points.

As we will see the topological degree and the index of an isolated solution are particularly well-suited instruments for obtaining results in this direction. Existence and non-existence theorems are easily stated and proved in terms of indices, without demanding anything else but continuity of $F(x,\lambda)$. In order to obtain more detailed information one is forced to use analytical tools which are constructive in nature. Then usually the mapping F is supposed to be differentiable, or even analytical, and results are stated in terms of derivatives.

In its generality the basic problem is far too difficult and too extensive (even in the finite-dimensional case) to be dealt with in this chapter. So we will make from time to time important restrictions. But first of all we prove a general theorem by means of simple topological arguments based on degree theory.

THEOREM 2.4. *If* λ_0 *is not a bifurcation point with respect to* Γ *then the index of* $x(\lambda)$ *is constant for all* λ *in some neighbourhood of* λ_0.

PROOF. Since $x(\lambda)$ depends continuously on λ, for every $\varepsilon > 0$ a $\delta(\varepsilon) > 0$ can be found such that $|\lambda - \lambda_0| < \delta(\varepsilon)$ implies $|x(\lambda) - x(\lambda_0)| < \varepsilon$. Assume λ_0 is not a bifurcation point. Then $\varepsilon > 0$ can be chosen such that any solution in the (n+1)-dimensional ball with radius ε and origin $(x(\lambda_0),\lambda_0)$ lies on Γ. So for $|\lambda - \lambda_0| < \eta = \min(\varepsilon,\delta(\varepsilon))$ there are no solutions (x,λ) with $|x - x(\lambda_0)| = \varepsilon$, and from theorem II.3.4 it follows that $\deg(F(.,\lambda),\Omega,0)$ is constant for $|\lambda - \lambda_0| < \eta$. Here Ω denotes the open ball $\{x \mid |x - x(\lambda_0)| < \varepsilon\}$. Since for a given value λ with $|\lambda - \lambda_0| < \eta$, $(x(\lambda),\lambda)$ is the only solution of (2.1) in Ω it follows from theorem II.3.14 that $\deg(F(.,\lambda),\Omega,0) = \mathrm{ind}(F(.,\lambda),x(\lambda),0)$. □

COROLLARY 2.5. *(A sufficient condition for a bifurcation point)*
Assume that every neighbourhood of the number λ_0 *contains two points* λ_1 *and* λ_2 *such that* $\mathrm{ind}(F(.,\lambda_1),x(\lambda_1),0) \neq \mathrm{ind}(F(.,\lambda_2),x(\lambda_2),0)$, *then* λ_0 *is a bifurcation point of* (2.1) *with respect to* Γ.

We conclude this section with three one-dimensional examples.

EXAMPLE 2.6. Define $F(x,\lambda) = ax + bx^2 - \lambda x$. One easily verifies by a homotopy argument that $\deg(F(.,\lambda),\Omega,0) = 0$, where Ω is a sufficiently large ball. Equation (2.1) has the two solution curves $\{(0,\lambda) \mid \lambda \in \mathbb{R}\}$ and $\{((\lambda-a)b^{-1},\lambda) \mid \lambda \in \mathbb{R}\}$ which intersect for $\lambda = a$. At the point of intersection the value of the indices are interchanged as sketched in figure 1 for a, b > 0.

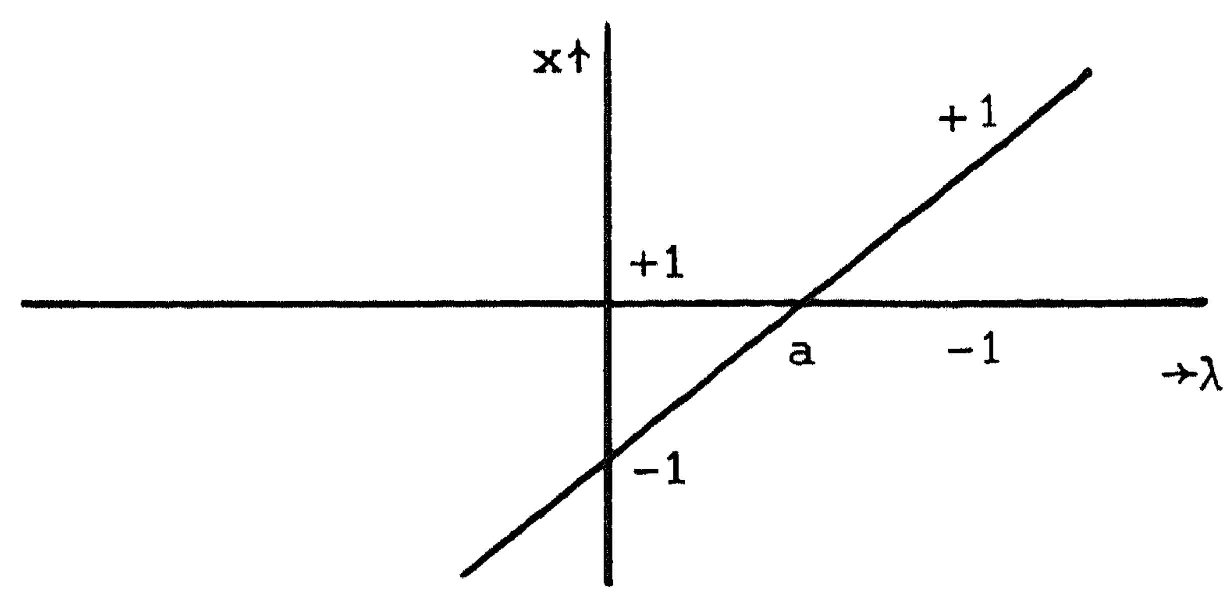


Figure 1

EXAMPLE 2.7. Suppose $F(x,\lambda) = ax^3 + bx - \lambda x$. There are two solution curves: $\{(0,\lambda) | \lambda \in \mathbb{R}\}$ and $\{(x,ax^2+b) | x \in \mathbb{R}\}$. The two curves intersect at $(0,b)$. For $a > 0$, $b > 0$ the situation is as in figure 2.

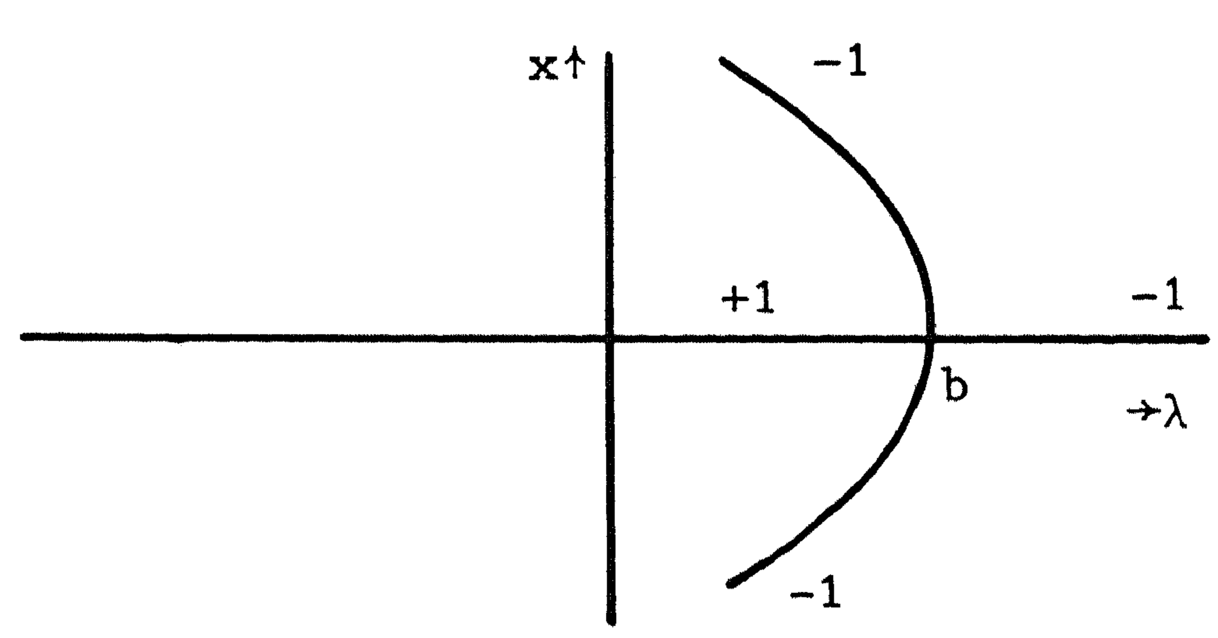


Figure 2

At the bifurcation point $\lambda = b$ the index of the simple curve $\{(0,\lambda) | \lambda \in \mathbb{R}\}$ changes. Note that the second curve is not simple.

EXAMPLE 2.8. Define $F(x,\lambda) = x(x^2-\lambda)\ (2x^2-\lambda)$. Solution curves and indices are easily calculated and they are sketched in figure 3.

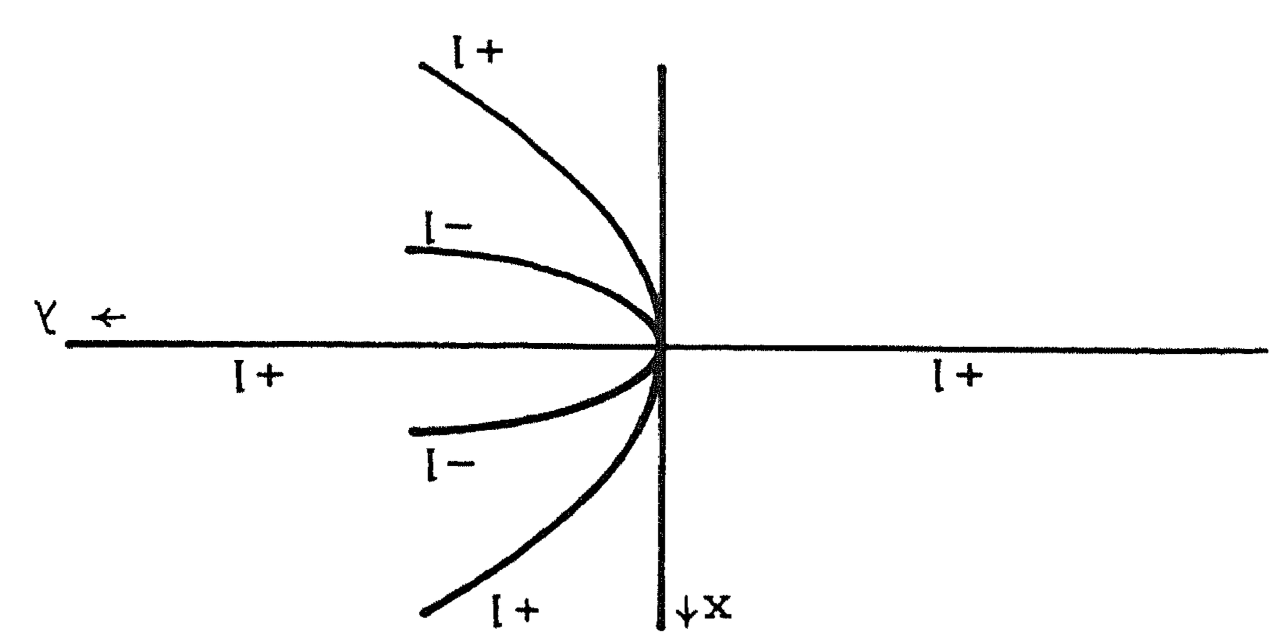


Figure 3

Note that the index x = 0 does not change at the bifurcation point $\lambda = 0$. So it is demonstrated that the sufficient condition of corollary 2.5 is not a necessary condition.

<u>REMARK 2.9</u>. Qualitative pictures such as the figures 1, 2 and 3 are called *bifurcation* (or *branching) diagrams*.

3. LINEARIZATION

In the present section a hypothesis concerning the function $F(x,\lambda)$ will enable us to obtain stronger results.

HYPOTHESIS 3.1. There exists a continuous differentiable function $f(x)$ such that $f(0) = 0$ and

$$(3.1) \qquad F(x,\lambda) = f(x) - \lambda x.$$

REMARK 3.2. A small remainder $R(x,\lambda)$ in (3.1) would not give rise to serious complications, but with the present restriction the calculations are carried out more easily and the applications we have in mind do meet (3.1).

Equation (2.1) can now be written as

$$(3.2) \qquad f(x) = \lambda x.$$

Henceforth the basic solution will be $\{(0,\lambda) \mid \lambda \in \mathbb{R}\}$ and a solution belonging to it will be called a *trivial solution*. So at first the problem is to find the values of λ for which there exist non-trivial solutions, i.e. solutions with $|x| \neq 0$, in every neighbourhood. A first result in this direction can be obtained from the well-known

THEOREM 3.3. *(Implicit function theorem)*
Let g *be a function defined on an open set* $\Omega \subset \mathbb{R}^n \times \mathbb{R}^k$ *with values in* $\mathbb{R}^n$. *Assume that*

(i) $g \in C^1(\Omega)$,

(ii) $g(x_0,y_0) = 0$,

(iii) *the Jacobian* nxn-*matrix representing* $g_x(x_0,y_0)$ *is non-singular (an equivalent statement is:* $g_x(x_0,y_0)\colon \mathbb{R}^n \to \mathbb{R}^n$ *has an inverse).*

Then there exist numbers $\varepsilon,\delta > 0$ *such that*

(1) *the neighbourhood* $V = \{(x,y) \mid |x-x_0| < \varepsilon,\ |y-y_0| < \delta\}$ *of* (x_0,y_0) *is contained in* Ω *and* $g_x(x,y)$ *has an inverse for every* $(x,y) \in V$,

(2) *for every* y *with* $|y-y_0| < \delta$ *there exists one and only one* $x = h(y)$ *with* $|x-x_0| < \varepsilon$ *such that* $g(x,y) = 0$,

(3) *the function* h *obtained in this way is continuous differentiable for* $|y-y_0| < \delta$ *and* $h'(y) = -\, g_x^{-1}(h(y),y)g_y(h(y),y)$.

A proof of this theorem can be found in DIEUDONNÉ [6, section X.2].

Returning to equation (3.2) we state the following

COROLLARY 3.4. *(A necessary condition for a bifurcation point)*
A number λ_0 *can be a bifurcation point of* (3.2) *only if* λ_0 *is an eigenvalue of* $f'(0)$.

PROOF. If λ_0 is not an eigenvalue of $f'(0)$ then $F_x(0,\lambda_0)$ has an inverse and by the implicit function theorem there exists a unique solution $(x(\lambda),\lambda)$ for $|\lambda-\lambda_0|$ sufficiently small. Since we know that $(0,\lambda)$ is a solution for every λ there can be no non-trivial solutions for $|\lambda-\lambda_0|$ sufficiently small. □

REMARK 3.5. $f'(0)x = \lambda x$ is called the *linearized equation* and the eigenvalues of $f'(0)$ are called the *eigenvalues of the linearized equation.* By definition the *spectrum* is the set of eigenvalues.

Knowing that bifurcation points are elements of the spectrum of the linearized equation, we might ask whether the reverse is true, that is, whether every eigenvalue of the linearized equation generates a bifurcation point. The answer is negative as follows from example 3.11 at the end of this section. It is, however, possible to obtain a sufficient condition by means of corollary 2.5.

But first we have to remind some definitions and results from linear algebra. Let A be an $n\times n$-matrix and μ an eigenvalue of A. The *algebraic multiplicity* of μ is defined as the multiplicity of μ as a zero of the characteristic polynomial. An eigenvalue is called *simple* if its algebraic multiplicity is equal to one. Denote the null space of a linear mapping L by $N(L)$, then clearly $N(L) \subset N(L^2)$. The *Riesz index* $r(\mu)$ is defined as the least integer k such that $N(A-\mu I_n)^{k+1} = N(A-\mu I_n)^k$. The subspace $N(A-\mu I_n)^{r(\mu)}$ is called the *generalized eigen-space* of the eigenvalue μ. A standard result of linear algebra states that the algebraic multiplicity is equal to the dimension of the generalized eigen-space. Finally, the *geometric multiplicity* of μ is defined as $\dim N(A-\mu I_n)$.

THEOREM 3.6. *(A sufficient condition for a bifurcation point)*
If λ_0 *is an eigenvalue of odd algebraic multiplicity of* $f'(0)$ *then* λ_0 *is a bifurcation point of* (3.2).

PROOF. Suppose λ_0 is not a bifurcation point. Then the index of the trivial solution remains constant for $|\lambda-\lambda_0|$ sufficiently small by theorem 2.4. From theorem II.3.13 we know that $\text{ind}(F(.,\lambda),0,0) = \text{sign}\det(f'(0)-\lambda I_n)$ and since λ_0 is an eigenvalue of odd algebraic multiplicity the index has to change sign as λ crosses λ_0. So we have a contradiction. □

The conclusion of theorem 3.6 can be extended somewhat. Since the eigenvalues form a discrete set we can find $\delta > 0$ such that $0 < |\lambda-\lambda_0| \le \delta$ implies λ is not an eigenvalue of $f'(0)$. Then by corollary 3.4, λ cannot be a bifurcation point for $0 < |\lambda-\lambda_0| \le \delta$. Choose $\eta > 0$ such that $F(x,\lambda) = 0$ has no non-trivial solutions for $\lambda = \lambda_0 \pm \delta$ and $|x| \le \eta$. Then

$$\begin{aligned}\deg(F(.,\lambda_0-\delta),\Omega,0) &= \text{ind}(F(.,\lambda_0-\delta),0,0)\\ &\ne \text{ind}(F(.,\lambda_0+\delta),0,0) = \deg(F(.,\lambda_0+\delta),\Omega,0),\end{aligned}$$

where Ω is any open set contained in the bal $\{x \mid |x| \le \eta\}$ and such that $0 \in \Omega$. But then for some value λ in the interval $(\lambda_0-\delta,\lambda_0+\delta)$ there has to be a solution of $F(x,\lambda) = 0$ with $x \in \partial\Omega$ (cf. theorem II.3.4), and we have shown that the non-trivial solutions have the property that the intersection with the boundary $\partial\Omega$ of each open set Ω containing zero and lying in a ball of sufficiently small radius, is non-empty. The set of non-trivial solutions is said to form a *continuous branch* near the bifurcation point λ_0.

The results we have obtained are local in nature. Rabinowitz has shown that bifurcation from an eigenvalue of odd multiplicity is a global rather than a local phenomenon. Again the basic tool is the degree of a mapping but the existence of non-trivial solutions is proved without limitation to small neighbourhoods. Define a *continuum* of solutions as a closed connected set $\{(x,\lambda)\}$ satisfying $F(x,\lambda) = 0$. The main result of Rabinowitz is the following theorem, for the proof of which we refer to the original article [7].

THEOREM 3.7. *If* λ_0 *is an eigenvalue of* $f'(0)$ *of odd algebraic multiplicity then there is a maximal continuum of solutions* Λ_0*, containing non-trivial solutions, such that* $(0,\lambda_0) \in \Lambda_0$ *and either* Λ_0 *tends to infinity in* $\mathbb{R}^n \times \mathbb{R}$ *or* Λ_0 *meets a point* $(0,\lambda_1)$*, where* λ_1 *is another eigenvalue of* $f'(0)$.

Having shown that the problem of finding the bifurcation points of a nonlinear equation can be simplified by studying the linearized equation, we will demonstrate this principle by means of some simple examples.

EXAMPLE 3.8. Consider the equation $1 - e^{-x} - \lambda x = 0$, $x,\lambda \in \mathbb{R}$.
Then $f(x) = 1 - e^{-x}$ and $f'(0)$ is the identity mapping. Clearly the only eigenvalue of $f'(0)$ is $\lambda = 1$, and it is necessarily simple. So if λ crosses $\lambda_0 = 1$ bifurcation must take place. The reader may verify this by finding the solutions graphically.

In the remaining examples n will be equal to two.

EXAMPLE 3.9. Let

$$f_1(x_1,x_2) = 8x_1 + 6x_1^3 + 12x_1x_2^2,$$
$$f_2(x_1,x_2) = 4x_2 + 3x_2^3 + 6x_2x_1^2,$$

then

$$f'(0) = \begin{pmatrix} 8 & 0 \\ 0 & 4 \end{pmatrix}.$$

From theorem 3.6 we conclude that $\lambda = 4$ and $\lambda = 8$ are bifurcation points. The non-trivial solutions of (3.2) are in fact easily expressed explicitly. Suppose $x_1 = 0$ then it follows that $x_2^2 = \frac{1}{3}(\lambda-4)$. Likewise we obtain for $x_2 = 0$, $x_1^2 = \frac{1}{6}(\lambda-8)$, whereas the assumption $x_1 \neq 0$, $x_2 \neq 0$ leads to $x_2^2 = -\frac{4}{9}$ which is impossible.

EXAMPLE 3.10. *(Secondary bifurcation)*
Next we look at

$$f_1(x_1,x_2) = 16x_1 + 12x_1^3 + 24x_1x_2^2,$$
$$f_2(x_1,x_2) = 12x_2 + 9x_2^3 + 18x_2x_1^2.$$

The bifurcation points are found to be $\lambda = 12$ and $\lambda = 16$ and the bifurcating branches are given by $x_1 = 0$, $x_2^2 = \frac{1}{9}(\lambda-12)$ and $x_2 = 0$, $x_1^2 = \frac{1}{12}(\lambda-16)$ respectively. But for $\lambda > 24$ we also have the non-trivial solution $x_1^2 = \frac{4}{9}(\frac{5\lambda}{48} - 1)$, $x_2^2 = \frac{4}{9}(\frac{\lambda}{24} - 1)$. The latter solution bifurcates from the solution curve $\{(\frac{1}{12}(\lambda-16),\lambda) \mid \lambda > 16\}$ and this phenomenon is called *secondary bifurcation.* The situation is illustrated in figure 4.

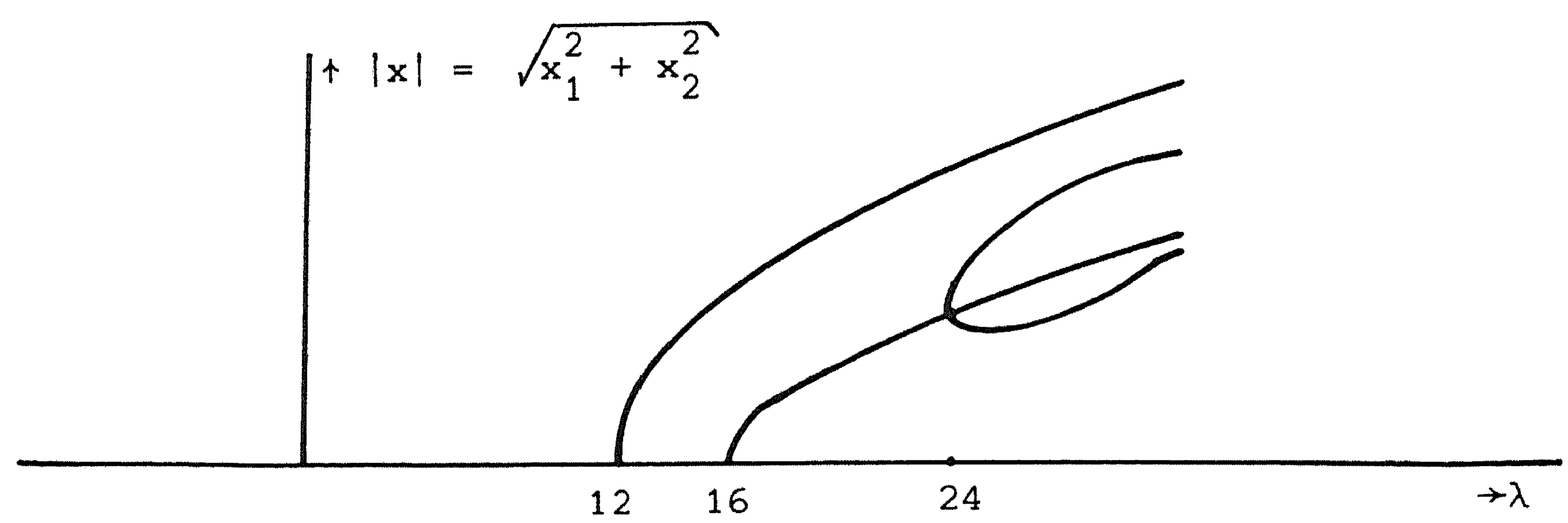


Figure 4

It is left to the reader to check that $\lambda = 24$ is an element of the spectrum of the equation obtained by linearizing $F(x,\lambda)$ about the solution curve from which the secondary bifurcation takes place. Finally, it is worth-while to notice that the functions f in this and the preceding example can be obtained from each other by multiplication with a constant factor.

In the examples presented thus far all eigenvalues were simple. The remaining examples will show that in the case of an eigenvalue of algebraic multiplicity greater than one a wide variety of possibilities may occur.

EXAMPLE 3.11. *(No bifurcation from a double eigenvalue)*
Let f(x) be defined by

$$f_1(x_1,x_2) = x_1^3 + x_2,$$
$$f_2(x_1,x_2) = x_1^2 x_2 - x_1^3.$$

Then

$$f'(0) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

showing that $\lambda = 0$ is a double eigenvalue. Equation (3.2) has no non-trivial solutions, for suppose

$$x_1(\lambda - x_1^2) = x_2 \quad ,$$
$$x_2(\lambda - x_1^2) = -x_1^3$$

and $x_1 > 0$, then it follows from the first equation that sign $x_2 = \text{sign}(\lambda - x_1^2)$, whereas from the second equation it follows that sign $x_2 = \text{sign}(x_1^2-\lambda)$. A similar contradiction is obtained by supposing $x_1 < 0$. Finally, if $x_1 = 0$ then the conclusion $x_2 = 0$ is immediate.

From theorem 2.4 we know that the index of the trivial solution has to remain constant as λ crosses zero. Explicitly we have $\text{ind}(F(.,\lambda),0,0) = \text{sign}\,\lambda^2$.

In the present example the geometric multiplicity of the double eigenvalue is equal to one.

<u>EXAMPLE 3.12</u>. *(A single branch emanating from a double eigenvalue)* Consider f(x) given by

$$f_1(x_1,x_2) = x_1 + 2x_1x_2 \qquad ,$$

$$f_2(x_1,x_2) = x_2 + x_1^2 + 2x_2^2.$$

Obviously $\lambda = 1$ is the only eigenvalue of the linearized equation. The set of non-trivial solutions consists of the line $\{(x,\lambda) \mid x_1 = 0,\ x_2 = \frac{1}{2}(\lambda-1),\ \lambda \in \mathbb{R}\}$. For all values of λ the trivial solution has index one and the non-trivial solution has index zero.

<u>EXAMPLE 3.13</u>. *(Two branches emanating from a double eigenvalue)* Suppose f(x) is defined by

$$f_1(x_1,x_2) = x_1 + ax_1(x_1^2+x_2^2),$$

$$f_2(x_1,x_2) = x_2 + \ x_2(x_1^2+x_2^2),$$

where the constant a is chosen to satisfy $a > 1$. $\lambda = 1$ is a double eigenvalue and the non-trivial solutions are found to be given by $x_1^2 = \frac{1}{a}(\lambda-1)$, $x_2 = 0$ and $x_1 = 0$, $x_2^2 = \lambda - 1$. The indices are noted in the bifurcation diagram figure 5.

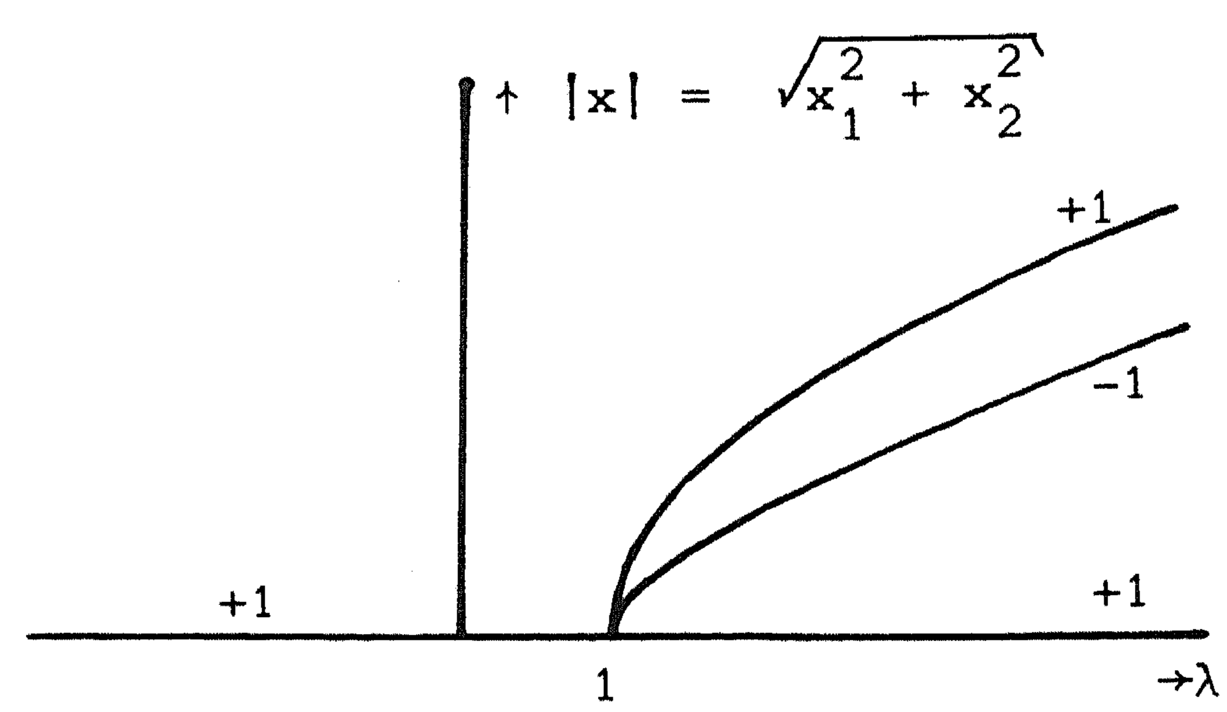


Figure 5

<u>EXAMPLE 3.14</u>. *(A continuum of branches emanating from a multiple eigenvalue)* Consider the preceding example but now with a equal to one. Then the problem of finding non-trivial solutions reduces to solving the single equation

$$x_1^2 + x_2^2 = \lambda - 1.$$

The solutions form the surface of a paraboloid of revolution about the λ-axis. Note that a bifurcation diagram of $|x|$ versus λ would not show the existence of the continuum of branches.

4. CONSTRUCTIVE METHODS

The examples presented thus far have in common that the bifurcating solutions can easily be found explicitly. This is due of course to the selection of examples we made. In general the bifurcating solutions are only implicitly defined.

In the present section we will discuss a method by which (2.1) is carried over into two simultaneous equations, the decomposition being such that, near the bifurcation point, one of the equations has a unique solution. In a special case the remaining second equation can be solved by elementary means. The method goes back to Lyapunov and Schmidt and it was developed as a tool in the study of nonlinear integral equations.

Again we will make some important hypotheses by which the generality of the problem is reduced. They will be stated at the moment they become essential.

4.1. PSEUDOINVERSE, DEFINITION AND APPLICATION

The starting-point is an equation

$$f(x) - \lambda x = 0, \qquad f \in C^1,\ f(0) = 0, \tag{4.1}$$

and an eigenvalue of $f'(0)$, λ_0 say. The goal is information about the solution set of (4.1) near $(0,\lambda_0)$.

First of all (4.1) will be written in a more suggestive way. Define

$$r(x) = f(x) - f'(0)x, \tag{4.2}$$

then of course $|r(x)| = o(|x|)$ as $|x| \to 0$. Furthermore, we write

$$\lambda = \lambda_0 + \tau \tag{4.3}$$

and

$$L = f'(0) - \lambda_0 I_n. \tag{4.4}$$

Then L is a linear mapping which is not invertible, and equation (4.1) is equivalent to

(4.5) $\quad Lx = h(\tau,x)$,

where

(4.6) $\quad h(\tau,x) = \tau x - r(x)$.

Now suppose the geometric multiplicity of λ_0 to be $k \le n$. Then the null space N of L has dimension k and the range R of L has dimension $n-k$. But the subspaces N and R need not be complementary (two subspaces M and E are said to be complementary if for every $x \in \mathbb{R}^n$ there are uniquely determined elements y and z of M and E respectively such that $x = y + z$; we then write $\mathbb{R}^n = M \oplus E$). In fact if the Riesz index $r(\lambda_0)$ is not equal to one, then for $y \in N(L^2)\backslash N$ it follows that $Ly \in N \cap R$.

By definition (4.5) has solutions if and only if $h \in R$, or equivalently, according to the well-known Fredholm alternative, $h \perp N^*$. Here N^* denotes the null space of L^*, the adjoint of L defined by $\langle y,Lz\rangle = \langle L^*y,z\rangle$ (in terms of real matrices the adjoint is the transpose). If h belongs to R, then there are many solutions, any two of which differ by an element of N.

Choose two subspaces M and E such that $\mathbb{R}^n = M \oplus N$ and $\mathbb{R}^n = E \oplus R$. Then we can define a linear mapping $L^{-1}: \mathbb{R}^n \to \mathbb{R}^n$, which is called a *pseudo-inverse* of L, by

$$L^{-1}h = y \quad \text{if } h = h_1 + h_2 \text{ with } h_1 \in E,\ h_2 \in R \text{ and}$$
$$y \in M \text{ is such that } Ly = h_2.$$

Note that indeed for $h_2 \in R$ the solution of $Ly = h_2$ is uniquely determined by the extra condition $y \in M$. The pseudoinverse depends on the choice of M and E. A possible choice is $M = N^\perp$ and $E = R^\perp$.

Define projections P and Q on N and M respectively ($Q = I-P$) and write for $x \in \mathbb{R}^n$, $x = p+q$ with $p = Px \in N$ and $q = Qx \in M$. Choose a basis $\phi_1^*,\dots,\phi_k^*$ for N^*. Then any solution of (4.5) must satisfy

(4.7a) $\quad \langle h(\tau,p+q),\phi_i^*\rangle = 0, \qquad i = 1,\dots,k,$

(4.7b) $\quad Lq = h(\tau,p+q)$.

Conversely, if $p \in N$ and $q \in M$ satisfy (4.7 a,b) then $x = p + q$ satisfies (4.5). The consistency condition (4.7a) is called the *bifurcation equation*. In view of (4.7a) we may apply the pseudoinverse to the left- and righthand side of (4.7b) yielding

$$(4.8) \qquad q = L^{-1}h(\tau,p+q).$$

So far nothing has been said about "small" solutions and in fact all transformations are valid without restriction. But the equation (4.8) can be written as

$$(4.9) \qquad G(q,p,\tau) = 0,$$

where $G\colon M \times N \times \mathbb{R} \to M$ is a C^1 mapping and $G_q(0,0,0)\colon M \to M$ is invertible. So from an obvious variant of theorem 3.3 we conclude the existence of a C^1 function $q = \hat{q}(\tau,p)$, such that $\hat{q}(\tau,p)$ is the only small solution of (4.9) for $\tau, |p|$ sufficiently small.

Finally, by substituting $q = \hat{q}(\tau,p)$ into (4.7a), we obtain k nonlinear equations in the unknowns τ and p, where τ is a scalar and p is an element of a k-dimensional subspace. Thus the original n-dimensional system reduces to a k-dimensional system. This last problem, which is in general quite complicated, falls outside the scope of this chapter. For a survey of methods by which results can be obtained we refer to SATHER [8].

4.2. LYAPUNOV-SCHMIDT EQUATIONS

The analysis of the foregoing subsection can be simplified somewhat in the special case of Riesz index one.

<u>HYPOTHESIS 4.1</u>. $r(\lambda_0) = 1$.

The hypothesis implies that R and N are complementary subspaces, so we can take $M = R$, $E = N$. Then P and Q are projections on N and R respectively.

<u>THEOREM 4.2</u>. L *commutes with* P *(hence with* Q*) and* (4.5) *is equivalent to the pair*

$$(4.10a) \qquad Ph(\tau,p+q) = 0,$$

$$(4.10b) \qquad Lq = Qh(\tau,p+q).$$

<u>PROOF</u>. $PLx = 0$ since $Lx \in \mathcal{R}$ and $LPx = 0$ because $Px \in N$. Applying P to (4.5) we obtain (4.10a) whereas (4.10b) is obtained by applying Q. The converse follows by adding (4.10a) and (4.10b). □

The equations (4.10a,b) are called the *Lyapunov-Schmidt equations*. As in subsection 4.1 it follows that (4.10b) has a unique small solution.

4.3. BIFURCATION FROM A SIMPLE EIGENVALUE

As a matter of fact our efforts have not yielded any concrete information concerning $F^{-1}(0)$ since we are still left with the k-dimensional bifurcation equation. In the special case $k = 1$ this problem becomes manageable.

<u>HYPOTHESIS 4.3</u>. The eigenvalue λ_0 is simple.

Choose vectors ϕ and ϕ^* in N and N^* respectively, such that $\langle\phi,\phi^*\rangle = 1$. Then $Px = \langle x,\phi^*\rangle\,\phi$. Now write

(4.11) $$\alpha = \langle x,\phi^*\rangle$$

and recall (4.6), then (4.10a,b) become

(4.12a) $$\alpha\tau - \langle r(\alpha\phi+q),\phi^*\rangle = 0,$$

(4.12b) $$Lq = \tau q - Qr(\alpha\phi+q).$$

Note that (4.12a) is a scalar equation.

We intend to solve τ and q as functions of α, but first some remarks on the construction of solutions are in order. The unique solution in theorem 3.3 can be constructed by the method of successive approximations, which in this case is equivalent to Newton's method. However, to obtain qualitative local information asymptotic approximations based on Taylor's formula are better suited. Therefore, we state an extension of theorem 3.3.

<u>THEOREM 4.4</u>. *If the assumptions of theorem* 3.3 *are verified, and if in addition* g *is m times continuous differentiable in* Ω, *then* h *is m times continuous differentiable in a neighbourhood of* y_0. *If* g *is analytic in* Ω *then* h *is analytic in a neighbourhood of* y_0.

For the proof of theorem 4.4 we again refer to DIEUDONNÉ [6, section X.2].

REMARK 4.5. For the actual construction of the Taylor expansion of h the method of undetermined coefficients can be employed. The derivatives of $g(h(y),y)$ of order up to m have to vanish at $y = y_0$. So the derivatives of $h(y)$ at $y = y_0$ can be found successively.

The next hypothesis we make concerns $r(x)$. We know $|r(x)| = o(|x|)$, but we need a sharper estimate.

HYPOTHESIS 4.6. $|r(x)| = O(|x|^2)$ and $r'(x) = O(|x|)$.

The latter statement has to be understood as $|r'(x)y| = o(|x|)$ for every $y \in \mathbb{R}^n$. Note that the hypothesis is trivially fulfilled if $f \in C^2$.

THEOREM 4.7. *There exists* $\varepsilon > 0$ *such that* (4.5) *has a solution*

$$\tau = \hat{\tau}(\alpha), \qquad x = \alpha\phi + \hat{q}(\alpha)$$

for $|\alpha| < \varepsilon$, *and this is the only non-trivial solution for* $|\tau|$, $|Px|$ *and* $|Qx|$ *sufficiently small. Moreover,* $\hat{\tau}$ *and* $\hat{q}$ *are continuous differentiable on* $(-\varepsilon,\varepsilon)$ *and* $\hat{\tau} = O(\alpha)$, $\hat{q} = O(\alpha^2)$, $\hat{q}' = O(\alpha)$ *for* $\alpha \to 0$.

PROOF. We know already that (4.5) is equivalent to the pair (4.12a,b) and that (4.12b) has a unique small solution $\hat{q}(\tau,\alpha)$ which is continuous differentiable. Since $Qr(\alpha\phi+q) = Qr(\alpha\phi) + Qr'(\alpha\phi)q + o(|q|)$ and since $L - \tau$ is invertible for τ sufficiently small, we conclude from the assumed asymptotic properties of $r(x)$ that $\hat{q}(\tau,\alpha) = O(\alpha^2)$. Likewise we obtain from

$$\left(L-\tau + Qr'(\alpha\phi+\hat{q})\right)\hat{q}_\tau = \hat{q},$$

$$\left(L-\tau + Qr'(\alpha\phi+\hat{q})\right)\hat{q}_\alpha = - Qr'(\alpha\phi+\hat{q})\phi,$$

the estimates $\hat{q}_\tau = O(\alpha^2)$, $\hat{q}_\alpha = O(\alpha)$.

Substitute $\hat{q}(\tau,\alpha)$ into (4.12a) then either $\alpha = 0$ or

$$(4.13) \qquad H(\tau,\alpha) = \tau - \frac{\langle r(\alpha\phi+\hat{q}),\phi^*\rangle}{\alpha} = 0.$$

Since $H_\tau(0,0)$ is the identity mapping (here the asymptotic estimates are used), the implicit function theorem may again be applied. Now with $\tau = \hat{\tau}(\alpha)$, the unique small solution of (4.13), and $\hat{q}(\alpha) = \hat{q}(\hat{\tau}(\alpha),\alpha)$ the results follow at once. □

<u>REMARK 4.8</u>. Since $|q| = O(\alpha^2)$ the mapping $\alpha \to |x(\alpha)|$ is invertible for α sufficiently small. So we can parameterize the solution with $|x|$ as well, and in fact this approach is very common in bifurcation problems.

4.4. INITIAL SHAPE AND INDICES

In theorem 4.7 an existence and uniqueness result is stated, but the method of proof is in fact constructive. The coefficients of a Taylor approximation of $\hat{\tau}$ and $\hat{q}$ can be calculated up to the order of differentiability of $r(x)$. Especially the first non-zero term in the Taylor approximation of $\hat{\tau}$ is important since from this term the initial shape of the bifurcating solutions follows.

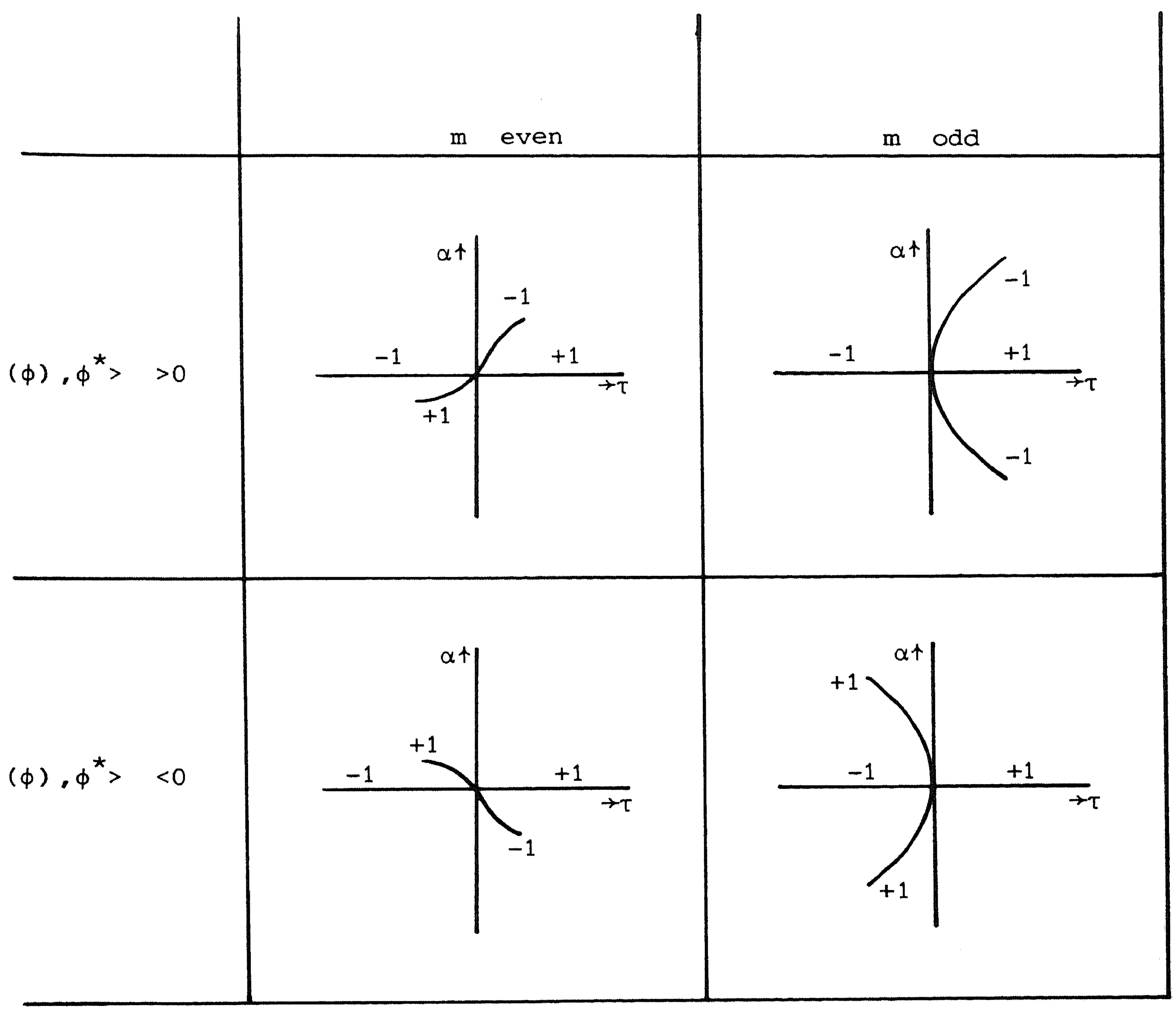
Now formally assume $f(x)$ to be many times continuous differentiable and suppose the first term in the expansion of $r(x)$ to be $f^m(0)x^m$, $m \geq 2$. Then, since $\hat{q} = O(\alpha^2)$, the first term in the expansion of $\hat{\tau}$ is found to be $\alpha^{m-1} \langle r(\phi),\phi^* \rangle$, and the initial shape follows from the signs of $\langle r(\phi),\phi^* \rangle$ and $(-1)^m$ (see figure 6). If $\langle r(\phi),\phi^* \rangle = 0$ we have to go to higher terms.

Clearly it may happen that $\hat{\tau}(\alpha) = 0$ for $|\alpha| < \delta < \varepsilon$. Then the bifurcation is said to be *vertical*. If $f(x)$ is linear the bifurcation is vertical but in the nonlinear case it can be as well.

We intend to determine the indices of the bifurcating solutions from the known index of the trivial solution. If the bifurcation is vertical then the index is not defined since solutions of $F(.,\lambda_0) = 0$ are not isolated. So again we make a hypothesis.

<u>HYPOTHESIS 4.9</u>. The bifurcation in λ_0 is not vertical.

Now for sufficiently small $\varepsilon > 0$ we can find $\delta(\varepsilon) > 0$ such that $|x| = \varepsilon$ and $|\tau| < \delta(\varepsilon)$ imply $F(x,\lambda_0+\tau) \neq 0$. Therefore, $\deg(F(.,\lambda_0+\tau),\Omega,0)$, where Ω is the open ball with radius ε, is defined and constant for $|\tau| < \delta(\varepsilon)$. In order to write the degree as a sum of indices all solutions have to be isolated. Although the bifurcation is not vertical, it is still possible that for every $\varepsilon > 0$ there are non-isolated solutions of $F(.,\lambda_0+\tau)$ with $|x| < \varepsilon$, $|\tau| < \delta(\varepsilon)$. By definition we call λ_0 a *regular bifurcation point* if there exists $\varepsilon > 0$ such that $\lambda_0 + \hat{\tau}(\alpha)$ is not in the spectrum of $f'(x(\alpha))$ for $0 < |\alpha| < \varepsilon$. The next theorem provides us with a useful criterion for a regular bifurcation point.



m even
m odd
$(\phi),\phi^*> \; >0$
$(\phi),\phi^*> \; <0$
$\alpha\uparrow$
$\rightarrow\tau$
-1
+1

Figure 6

<u>THEOREM 4.10</u>. λ_0 *is a regular bifurcation point if and only if there exists* $\varepsilon > 0$ *such that* $\hat{\tau}'(\alpha) \neq 0$ *for* $0 < |\alpha| < \varepsilon$.

<u>PROOF</u>. The notation is the same as in the proof of theorem 4.7. From $H(\hat{\tau}(\alpha),\alpha) = 0$ it follows that $H_\tau(\hat{\tau}(\alpha),\alpha)\hat{\tau}'(\alpha) + H_\alpha(\hat{\tau}(\alpha),\alpha) = 0$. Since $H_\tau(\tau,0) = 1$ we have $H_\tau(\tau,\alpha) \neq 0$ for α sufficiently small. So $\hat{\tau}'(\alpha) \neq 0$ if and only if $H_\alpha(\hat{\tau}(\alpha),\alpha) \neq 0$ or equivalently

$$\tau - \langle r'(\alpha\phi+\hat{q})\phi,\phi^*\rangle - \langle r'(\alpha\phi+\hat{q})\hat{q}_\alpha,\phi^*\rangle \neq 0.$$

On the other hand we have that $\lambda_0 + \hat{\tau}(\alpha)$ is in the spectrum of $f'(x(\alpha))$ if and only if there exists $v \neq 0$ such that $(L-\tau + r'(x(\alpha)))v = 0$. Write $v = \beta\phi + g$ with $g \in R$ and apply the projection Q. Then

$$(L-\tau + Qr'(x(\alpha)))g = - Qr'(x(\alpha))\beta\phi,$$

and this is true if and only if $g = \beta\hat{q}_\alpha$ and thus $v = \beta x(\alpha)$. Likewise application of P yields

$$- \tau\beta + \langle r'(x(\alpha))\beta x(\alpha),\phi^*\rangle = 0,$$

and this is true if and only if

$$\tau - \langle r'(\alpha\phi+\hat{q})\phi,\phi^*\rangle - \langle r'(\alpha\phi+\hat{q})\hat{q}_\alpha,\phi^*\rangle = 0. \qquad \square$$

<u>REMARK 4.11</u>. If $\hat{\tau}'(\alpha) \neq 0$ for $0 < |\alpha| < \varepsilon$ we can invert $\hat{\tau}(\alpha)$ and each subbranch can be expressed as a continuous differentiable function of λ.

<u>HYPOTHESIS 4.12</u>. λ_0 is a regular bifurcation point.

Now ε can be chosen such that all solutions of $F(.,\lambda_0+\tau) = 0$ with $|x| < \varepsilon$ are isolated and have index plus or minus one. Since the index of the trivial solution changes sign at $\tau = 0$ and since the sum of indices has to remain constant, the indices of the non-trivial solutions follow at once. In figure 6 the case where the trivial solution has index minus one for $\tau < 0$ is shown. The other possibility is obtained by multiplying all indices with minus one.

5. STABILITY OF BIFURCATING SOLUTIONS

In the introduction the study of the solution set of $F(x,\lambda) = 0$ was motivated by the interpretation of $F(x,\lambda)$ as the right-hand side of a differential equation for x. At first sight, our results so far seem hardly useful in connection with differential equations, but in this section our domain of interest is extended to stability of solutions, and our previous results will turn out to be applicable very well.

5.1. DEGREE THEORY AND LINEARIZED STABILITY

In chapter III section 3.4.2 the famous Poincaré-Lyapunov theorem was discussed. This theorem asserts the validity of the *principle of linearized stability*. So we have on the one hand a connection between the eigenvalues of the Jacobian matrix and stability, on the other hand we have a connection between the index and the eigenvalues (see theorem II.3.13). This is the keystone for the application of degree theory to stability analysis, and it forms the basis of some results in chapter III (cf. theorem III.3.19). In the case of regular bifurcation from a simple eigenvalue the relation between the index and stability becomes particularly simple, and stronger results are possible (see SATTINGER [9] for the original results).

If the solutions of $F(x,\lambda) = 0$ are the steady states of some physical system, then a particular interesting situation occurs if the trivial solution is stable for λ less than some critical value λ_0, but becomes unstable when λ is increased beyond λ_0. In this connection non-trivial solutions for $\lambda > \lambda_0$ are called *supercritical* and non-trivial solutions for $\lambda < \lambda_0$ *subcritical*.

THEOREM 5.1. *Subcritical branches are unstable, supercritical branches are stable.*

PROOF. In section 4 it was shown that the bifurcating solutions constitute two subbranches which meet only at $(0,\lambda_0)$. Denote one of them by $x(\lambda)$. Then $x(\lambda)$ is defined on an interval J, with either $J = [\lambda_0,\lambda_0+\delta)$ or $J = (\lambda_0-\delta,\lambda_0]$. Denote the eigenvalues of $f'(0) - \lambda I_n$ by $\mu_1(\lambda),\ldots,\mu_n(\lambda)$ and those of $f'(x(\lambda)) - \lambda I_n$ by $\sigma_1(\lambda),\ldots,\sigma_n(\lambda)$. The eigenvalues are continuous functions of λ and so for $\lambda \to \lambda_0$ we have $\sigma_i(\lambda) \to \mu_i(\lambda_0)$, $i = 1,\ldots,n$. Since λ_0 is a simple eigenvalue of $f'(0)$, one of the eigenvalues, μ_1 say, has to be zero for $\lambda = \lambda_0$, and there exists $\varepsilon_1 > 0$ such that for $|\lambda-\lambda_0| < \varepsilon_1$ $\mu_1(\lambda)$ is real and for $\lambda \in J$ also $\sigma_1(\lambda)$ is real (recall that nonreal eigenvalues occur in complex conjugate pairs only). From the assumed stability of the trivial solution it follows that Re $\mu_i(\lambda_0) < -\delta' < 0$, $i = 2,3,\ldots,n$ and hence there exists $\varepsilon_2 > 0$ such that Re $\mu_i(\lambda) < -\frac{\delta'}{2} < 0$ and Re $\sigma_i(\lambda) < -\frac{\delta'}{2}$ for $\lambda \in J$ and $|\lambda-\lambda_0| < \varepsilon_2$. Therefore, for $\lambda \in J$ sufficiently close to λ_0 we have

$$\text{sign } \mu_2(\lambda) \ldots \mu_n(\lambda) = \text{sign } \sigma_2(\lambda) \ldots \sigma_n(\lambda).$$

In section 4 we showed that

$$\text{ind}(F(.,\lambda),x(\lambda),0) = -\text{ ind}(F(.,\lambda),0,0)$$

and thus

$$\text{sign } \mu_1(\lambda)\mu_2(\lambda) \ldots \mu_n(\lambda) = -\text{ sign } \sigma_1(\lambda)\sigma_2(\lambda) \ldots \sigma_n(\lambda).$$

Therefore, $\mu_1(\lambda)$ and $\sigma_1(\lambda)$ must have opposite signs. □

<u>REMARK 5.2</u>. Theorem 5.1 can be proved by perturbation methods as well. Then the first term in a formal perturbation series for the critical eigenvalue has to be calculated. But the success of this approach depends on the non-vanishing of coefficients and the procedure is rather technical.

<u>REMARK 5.3</u>. From a mathematical point of view the restriction to bifurcation from a stable trivial solution is rather inessential. Suppose the trivial solution to be a saddle point of type (k) for $\lambda < \lambda_0$ (i.e., all eigenvalues of $f'(0) - \lambda I_n$ have nonzero real parts, k of which are negative). Then with both the trivial solution and the bifurcating solutions we can associate stable and unstable manifolds (see HALE [10, section III.6]) and the contents of theorem 5.1 can be expressed in terms of dimensions of these manifolds.

5.2. CONTINUOUS-FLOW STIRRED TANK REACTORS

In chapter III a model for a chemical system involving both transport and chemical reactions was discussed. For such an open system the conservation equations for the chemical species are written as (cf. (2.6) on p.45)

$$(5.1) \qquad \frac{dc}{dt} = \frac{1}{\theta}(c_f-c) + \nu^T f(c).$$

The first term on the right-hand side is due to input and output streams, whereas the second is a source term due to chemical reactions. The holding time θ is a characteristic quantity for the mutual proportion of transport and reactions. From the definition (cf. p.45) it follows that the constant θ is adjustable.

We consider the case of constant inflow, i.e., the feed state c_f is a constant vector. As in section III.4 we define

$$(5.2) \qquad c - c_f = \nu^T\xi, \qquad \xi \in \mathbb{R}^r,$$

and we study henceforth the steady state equation

$$(5.3) \qquad \tilde{f}(\xi) - \frac{1}{\theta}\,\xi = 0.$$

A question that arises naturally from the discussion of closed and open systems in chapter III is the following. Suppose the feed state c_f is an equilibrium solution of the corresponding closed system, then c_f is a steady state also. But how about the stability of c_f as a steady state? Does the stability depend on θ? If it does, what happens in case of transition to instability? Are there steady states close to c_f?

Mathematically this means we are assuming $\tilde{f}(0) = 0$ in (5.3) and we are interested in bifurcation as θ varies. Hence the question fits the framework of this chapter and we underline this by writing

$$(5.4) \qquad \frac{1}{\theta} = \lambda, \quad \xi = x, \quad \tilde{f} \to f.$$

Moreover, we assume f to be continuous differentiable.

The theory of the foregoing sections enables us to give immediately a partial answer to the question. From corollary 3.4 we know that bifurcation points are elements of the spectrum of the linearized equation, and from theorem 3.6 it follows that every simple eigenvalue is indeed a bifurcation point. Now suppose that c_f is a stable equilibrium point, then all eigenvalues of $f'(0)$ have negative real part and since λ is positive the eigenvalues of $f'(0) - \lambda I_r$ share this property. Hence c_f is a stable steady state for all values of λ.

Suppose on the contrary that c_f is an unstable equilibrium point, then at least one of the eigenvalues of $f'(0)$ has positive real part. Denote by

λ_0 the eigenvalue with greatest positive real part and assume λ_0 is real and simple. Then bifurcation takes place as λ crosses λ_0. The steady state c_f is stable for $\lambda > \lambda_0$ and unstable for $\lambda < \lambda_0$. Moreover, theorem 5.1 holds.

REMARK 5.4. One might ask what happens if two complex conjugate eigenvalues of $f'(0) - \lambda I_r$ cross the imaginary axis, for then clearly the stability character of the trivial solution changes as well. This question falls outside the scope of this chapter but it is the subject of the following one.

Next we present two concrete examples. The first is one-dimensional and the emphasis is on gemometric interpretation. The second is two-dimensional and it serves as an exercise in the application of the techniques of section 4.

EXAMPLE 5.5. Let the graph of f(x) have the form shown in figure 7.

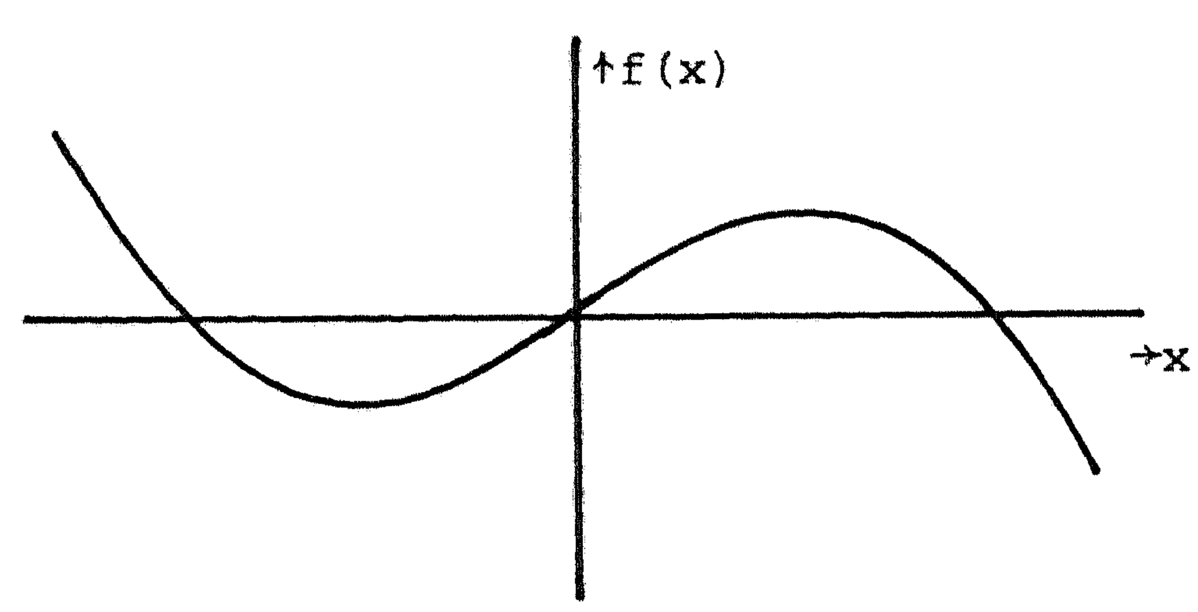


Figure 7

The solutions of (5.3) are the points of intersection of the graph of $f(x)$ with the line λx. We have bifurcation of the trivial solution $x = 0$ as the tangent of $f(x)$ at $x = 0$ coincides with λx. The initial shape of the bifurcating solutions can be found from a more detailed geometric inspection, but this is left to the reader.

Assume f to be many times differentiable. Analytically we have as a condition for bifurcation $f'(0) = \lambda$, and by writing $r(x) = f(x) - f'(0)x$, $\lambda = f'(0) + \tau$, we obtain the equation $\tau x = r(x)$. The solutions are $x = 0$ and $\tau = r(x)x^{-1}$. The latter solution can be expanded formally

$$\tau = \frac{f''(0)}{2!} x + \frac{f'''(0)}{3!} x^2 + \dots ,$$

and some possibilities are illustrated in figure 8 together with the corresponding stability character.

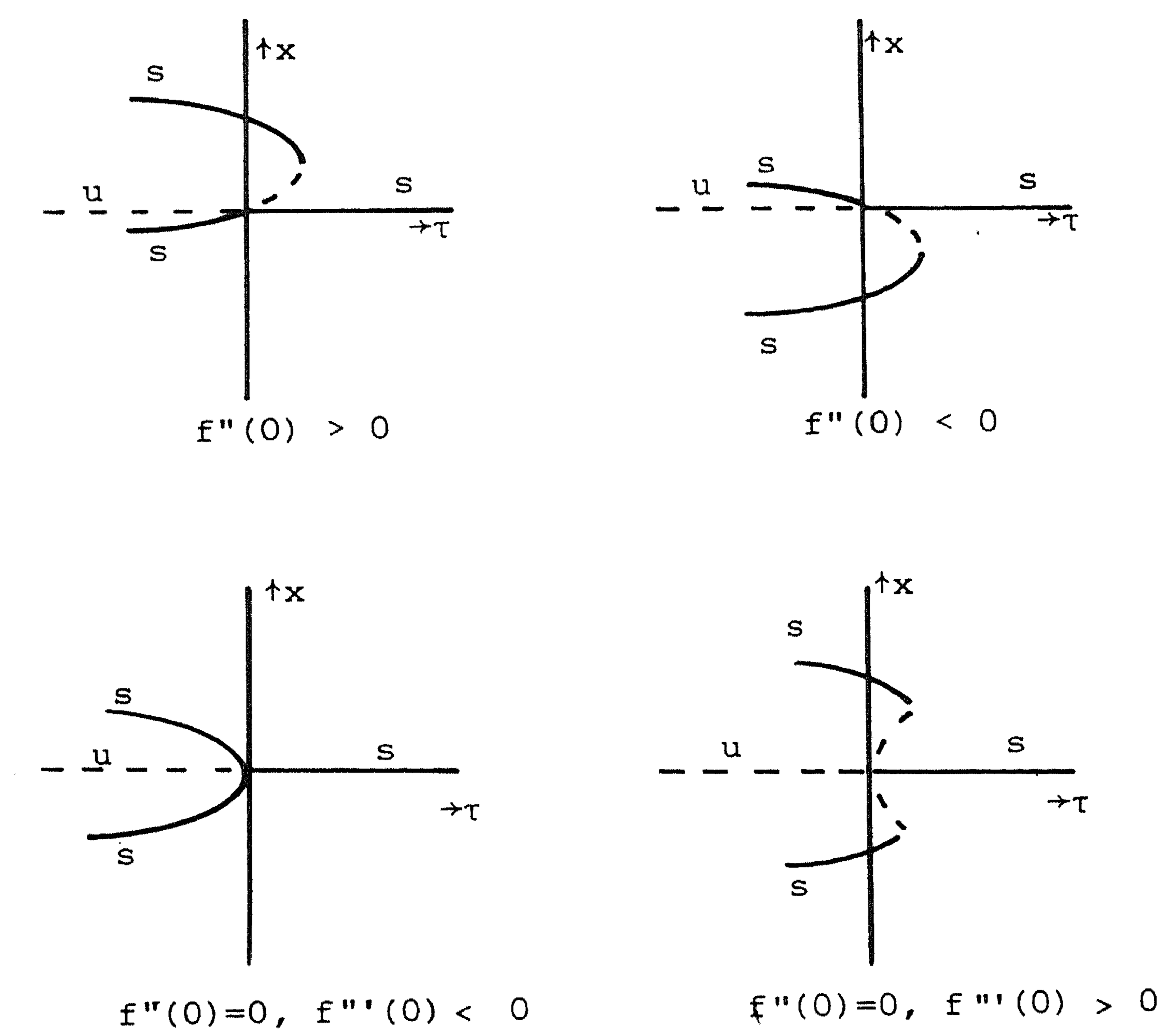


Figure 8

<u>EXAMPLE 5.6</u>. In example III.1.1 and example III.3.6 the reactions

$$2NO_2 - N_2O_4 = 0,$$

$$2NO + O_2 - 2NO_2 = 0,$$

were considered. Now let the rate functions be given by

$$f_1 = k_1\, c_3^2 - k_2\, c_4,$$

$$f_2 = k_3\, c_1\, c_2^2 - k_4\, c_3^2,$$

with

$$k_1 = 1, \quad k_2 = 5, \quad k_3 = \frac{9}{8}, \quad k_4 = 1,$$

and consider the open system with feed state

$$c_f = \begin{pmatrix} \frac{1}{2} \\ \frac{2}{3} \\ \frac{1}{2} \\ \frac{1}{20} \end{pmatrix} .$$

Then indeed $f_1(c_f) = f_2(c_f) = 0$. In terms of the extent vector x defined by $\nu^T x = c - c_f$ the steady state equation becomes

$$7x_1 - 2x_2 + 4(x_1-x_2)^2 - \lambda x_1 = 0,$$

$$- 2x_1 + 4x_2 - 4(x_1-x_2)^2 + 5\tfrac{1}{4}x_2^2 + 4\tfrac{1}{2}x_2^3 - \lambda x_2 = 0.$$

Clearly,

$$f'(0) = \begin{pmatrix} 7 & -2 \\ -2 & 4 \end{pmatrix} ,$$

and the eigenvalues are $\lambda_0 = 8$, $\lambda_1 = 3$. Hence the steady state $x = 0$ is stable for $\lambda > 8$, but becomes unstable as λ crosses the simple eigenvalue $\lambda_0 = 8$.

The null space N of the linear mapping

$$L = f'(0) - \lambda_0 I_2 = \begin{pmatrix} -1 & -2 \\ -2 & -4 \end{pmatrix}$$

is spanned by the unit vector

$$\phi = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ -1 \end{pmatrix},$$

and since L is self-adjoint (i.e., symmetric in the case of real matrices) ϕ is a basis vector for the subspace N^* as well. The range R of L is spanned by the unit vector

$$\psi = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix},$$

and the projection Q on $\mathcal{R}$ is defined by $Qx = \langle x,\psi\rangle\psi$.

Furthermore, we have, with $h(\tau,x) = \tau x - r(x) = \tau x - (f(x)-f'(0)x)$,

$$h_1(\tau,x) = \tau x_1 - 4(x_1-x_2)^2,$$

$$h_2(\tau,x) = \tau x_2 + 4(x_1-x_2)^2 - 5\tfrac{1}{4}x_2^2 - 4\tfrac{1}{2}x_2^3.$$

Now with $\tau = \lambda - \lambda_0$, $\alpha = \langle x,\phi\rangle = \frac{1}{\sqrt{5}}(2x_1-x_2)$, $\beta = \langle x,\psi\rangle = \frac{1}{\sqrt{5}}(x_1+2x_2)$, the steady state equation can be written as (compare (4.12a,b))

$$\alpha\tau - \frac{12}{\sqrt{5}}\left(\frac{3\alpha-\beta}{\sqrt{5}}\right)^2 + \frac{5\frac{1}{4}}{\sqrt{5}}\left(\frac{2\beta-\alpha}{\sqrt{5}}\right)^2 + \frac{4\frac{1}{2}}{\sqrt{5}}\left(\frac{2\beta-\alpha}{\sqrt{5}}\right)^3 = 0,$$

$$-5\beta = \tau\beta + \frac{4}{\sqrt{5}}\left(\frac{3\alpha-\beta}{\sqrt{5}}\right)^2 - \frac{10\frac{1}{2}}{\sqrt{5}}\left(\frac{2\beta-\alpha}{\sqrt{5}}\right)^2 - \frac{9}{\sqrt{5}}\left(\frac{2\beta-\alpha}{\sqrt{5}}\right)^3 ,$$

or, equivalently,

$$-100\alpha\tau + 411\sqrt{5}\alpha^2 - 204\sqrt{5}\alpha\beta - 36\sqrt{5}\beta^2 + 18\alpha^3 - 108\alpha^2\beta + 216\beta^2\alpha - 144\beta^3 = 0,$$

$$-250\beta = 50\tau\beta + 51\sqrt{5}\alpha^2 + 36\sqrt{5}\alpha\beta - 76\sqrt{5}\beta^2 + 18\alpha^3 - 108\alpha^2\beta + 216\beta^2\alpha - 144\beta^3.$$

The latter equation can be solved for β as a function of α and τ. Substitute

$$\beta = \sum_{\substack{k,\ell=0\\ k+\ell\neq 0}}^{\infty} c_{kl}\tau^k\alpha^l$$

and equate coefficients. We obtain

$$\beta = -\frac{51}{250}\sqrt{5}\alpha^2 + \frac{51}{1250}\sqrt{5}\alpha^2\tau + \frac{468}{6250}\alpha^3 + \dots .$$

Notice that indeed $\beta = O(\alpha^2)$. The former equation yields $\alpha = 0$ or

$$-100\tau + 411\sqrt{5}\alpha - 204\sqrt{5}\beta - 36\sqrt{5}\beta^2\alpha^{-1} + 18\alpha^2 - 108\alpha\beta +$$
$$+ \ 216\beta^2 - 144\beta^3\alpha^{-1} = 0,$$

or, after substitution of the power series for β,

$$\tau = \frac{1}{100}\{411\sqrt{5}\alpha + \frac{5652}{25}\alpha^2 + \ldots\}.$$

Finally, the results in terms of α, β and τ can be translated into results in terms of x_1, x_2 and λ be executing all transformations backwards. Qualitatively the outcome is sketched in figure 9.

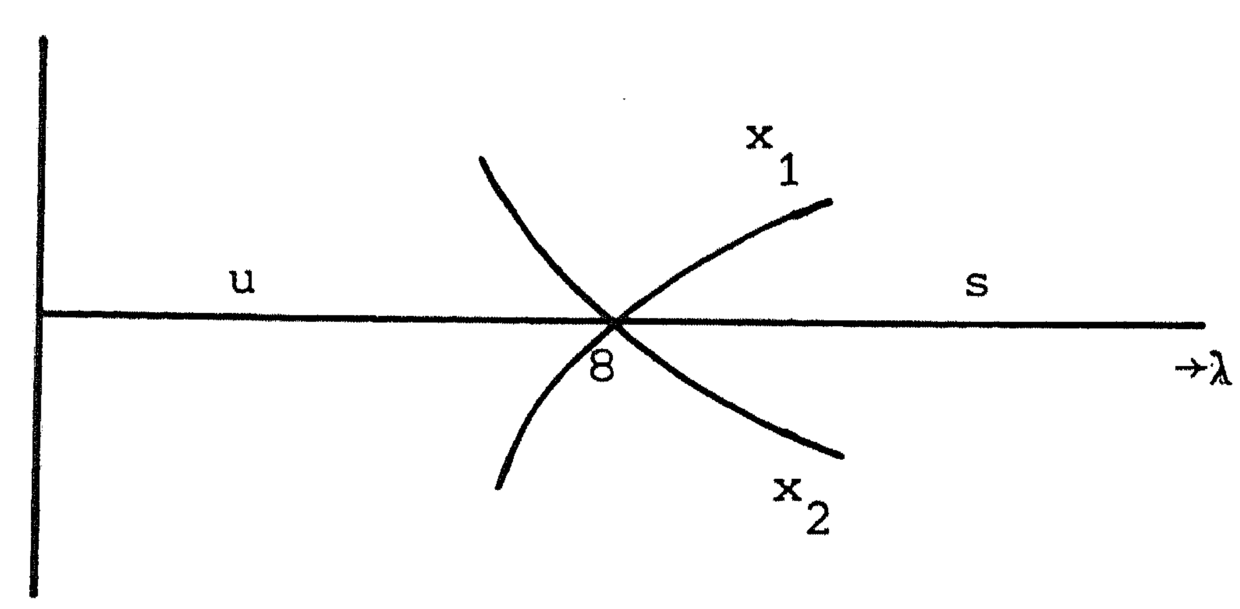


Figure 9

The non-trivial solution is unstable for $\lambda > 8$ and stable for $\lambda < 8$. If required, the concentrations c_1, c_2, c_3 and c_4 can be calculated from $c - c_f = \nu^T x$.

From a chemical engineering point of view our discussion of the continuous-flow stirred tank reactor is rather incomplete and the examples are artificial. The following remarks are intended to show that the analysis is applicable to more realistic systems as well. Consider an open system and regard the temperature T of the system as a state variable. In commonly encountered situations the reactions are controlled by a cooling mechanism and, in a first approximation, the cooling is proportional to the deviation of the reactor temperature from that of a desired temperature (for instance if a cooling fluid of constant temperature is used).

Consider one reaction, then the differential equations look like (cf. GAVALAS [11, p.29] and ARIS & ADMUNDSON [12])

$$\frac{dx}{dt} = -\frac{1}{\theta}x + F(x,T),$$

$$\frac{dT}{dt} = \frac{1}{\theta}(T_f - T) + KF(x,T) + Q(T).$$

The constant K is a measure for the heat produced by the reaction, and Q(T) is the amount of heat per unit time which is exchanged with the cooling fluid. The steady states follow from

$$x = \theta F(x,T),$$

$$K\theta F(x,T) = T - T_f - \theta Q(T).$$

For fixed θ the first equation can be solved for x as function of T. As pointed out by ARIS & ADMUNDSON [12] the result is generally sigmoid in shape. Next we solve the second equation graphically in the special case $Q(T) = 0$.

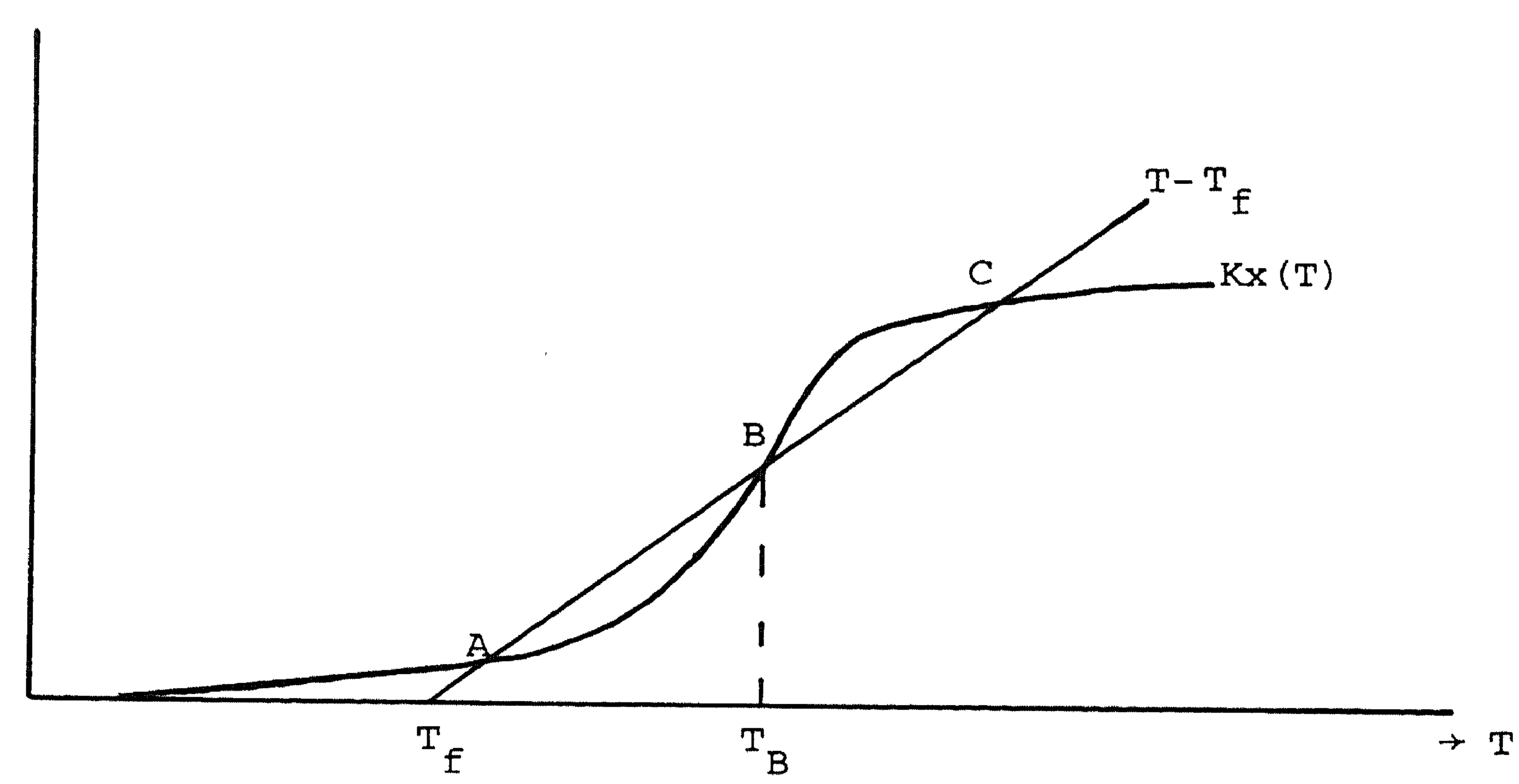


Figure 10

As in figure 10 there usually are three steady states A, B and C. Clearly the steady state B is unstable. However, the naturally unstable steady state B might be interesting from an industrial point of view. So suppose the function Q(T) is given by

$$Q(T) = \lambda(T_B - T), \quad \lambda > 0.$$

The steady state equation becomes

$$Kx(T) = (1+\theta\lambda)T - T_f - \theta\lambda T_B.$$

The right-hand side corresponds to a straight line through B with slope $1 + \theta\lambda$. For λ sufficiently large B is the only steady state and B is stable. If λ decreases B becomes unstable as $\theta\lambda$ crosses $Kx'(T_B) - 1$. It should be clear that this kind of problems can be analysed in more detail by the methods described in this chapter.

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V. BIFURCATION OF PERIODIC SOLUTIONS AND A MATHEMATICAL MODEL FOR THE STRUGGLE BETWEEN ANTIGEN AND ANTIBODY

In the present chapter we give an example of branching of a set of periodic solutions from a constant solution of a differential equation. This happens when the stability character of the constant solution changes by virtue of a complex conjugate pair of simple eigenvalues of the linearized equation crossing the imaginary axis. As general references for this chapter we mention BELL [1] and PIMBLEY [2] and [3].

1. INTRODUCTION

Since their introduction by Volterra and Lotka, simple mathematical models of interacting populations have been of interest not only because of the mathematical problems they pose, but also because they may indicate important features of the interactions and how these are reflected in temporal variations of the populations.

The infection of an animal with replicating material, such as bacteria, foreign cells, or virus, may produce an immune response. The foreign material provoking the response is called antigen and the immune response itself is characterized by the production of antibodies which are molecules that specifically bind to the antigen and hasten its destruction and repulsion by the animal. Apparently the antibodies are produced by certain cells in the animal which recognize the antigen as foreign material and are thereby stimulated to produce antibodies. For biological details see BELL [1] and references in this paper.

The immune response to a replicating antigen may be viewed as a problem with interacting populations of antigen, antibodies, and the cells which are involved in the production and in the effects of the antibodies. A detailed representation of such an immune response would be exceedingly complex; many different kinds of cells are involved and the antibody population is quite heterogeneous.

In this chapter we consider a simple model involving two populations. As a mathematical tool to prove the existence of a branch of periodic solutions in the neighbourhood of an equilibrium point we use a theorem of Friedrichs (section 3). In section 6 we describe the possibilities of the existence of periodic solutions in the two-dimensional case using the Poincare-Bendixson theorem, which is given in section 3. In section 7 we discuss our results in biological terms and we give some remarks on a three-dimensional case.

2. THE MATHEMATICAL MODEL AND APPROXIMATE EQUATIONS

This section is devoted to a model involving two populations, namely the antigens and the antibodies; antigen plays the role of prey and antibody the role of predator. Let A_g denote the concentration of antigen and A_b the concentration of antibody. We make the following assumptions.

ASSUMPTION 2.1. Each unit of antigen has only a single site for binding antibody, and each antibody can bind only a single antigen site.

ASSUMPTION 2.2. When antibody is not present the antigens will replicate and multiply in number with a rate constant λ_1.

ASSUMPTION 2.3. If an antigen is bound to an antibody, it will be eliminated with the rate constant α_1.

Thus, if $(A_g)_b$ denotes the concentration of bound antigen, we have as a first equation

$$(2.1a) \qquad \frac{dA_g}{dt} = \lambda_1 A_g - \alpha_1 (A_g)_b .$$

An equation as simple as the above equation for the antibody is much less obvious since in fact the antibodies are produced by cells which have been stimulated by antigen.

ASSUMPTION 2.4. In the absence of antigen the antibody concentration will decay with rate constant λ_2, while binding of antigen to antibody stimulates the production of antibody with rate constant α_2. In addition, the capacity of an animal to produce antibodies is clearly limited.

Let θ denote a limiting antibody concentration which cannot be exceeded by the animal. Then we present as a second equation

$$(2.1b) \qquad \frac{dA_b}{dt} = -\lambda_2 A_b + \alpha_2 (A_b)_b \; (1 - A_b/\theta),$$

where $(A_b)_b$ denotes the concentration of bound antibodies.

So far, we have introduced 4 state variables A_g, A_b, $(A_g)_b$ and $(A_b)_b$, and two differential equations. The remaining two relations between the state variables follow from assumption 2.1, which insures that

$$(2.2) \qquad (A_g)_b = (A_b)_b$$

and from the following assumption.

ASSUMPTION 2.5. There is chemical equilibrium between bound and free antigens and antibodies. The binding has an association constant k and the law of mass action states that

$$(2.3) \qquad (A_g)_b = (A_b)_b = k\{A_g - (A_g)_b\}\{A_b - (A_b)_b\}.$$

It may be noted that $A_g - (A_g)_b$ and $A_b - (A_b)_b$ are the concentrations of unbounded antigens and antibodies respectively.

By writing (2.3) in the form

$$(2.4) \qquad (A_b)_b = \frac{kA_bA_g}{1+k(A_b+A_g)-k(A_b)_b}$$

and by neglecting the last term in the denominator we obtain the approximation

$$(2.5) \qquad (A_b)_b^* = \frac{kA_bA_g}{1+k(A_b+A_g)}\ .$$

The error made in using (2.4) will be to underestimate $(A_b)_b$, but never by more than a factor 2. This follows from the following lemma.

LEMMA 2.6. *Let* $(A_b)_b$ *and* $(A_b)_b^*$ *be given as in* (2.4) *and* (2.5) *respectively. Then for any positive value of* k *we have*

$$\tfrac{1}{2}(A_b)_b \leq (A_b)_b^* \leq (A_b)_b.$$

PROOF. $(A_b)_b$ can be solved from the quadratic equation given in (2.4) and it is given by

$$(A_b)_b = \frac{2kA_gA_b}{1+k(A_g+A_b)+k\{(A_g+A_b+1/k)^2-4(A_gA_b)\}^{\frac{1}{2}}}\ ,$$

from which the proof easily follows. □

REMARK 2.7. If k is small, then, as follows from (2.4) and (2.5), we have

$$(A_b)_b = (A_b)_b^* \,(1+O(k)), \qquad k \to 0.$$

In the remaining part of this chapter the quantities $(A_b)_b$ and $(A_b)_b^*$ are identified with each other. The resulting differential equations share certain qualitative features with the differential equations we should obtain if we were to use the exact expression for $(A_b)_b$. They have the same number, kind and arrangement of singular points. They suffice for a qualitative investigation.

On letting

$$kA_b = x, \quad kA_g = y, \quad k\theta = \gamma^{-1}$$

(2.1a,b) will be written as

$$\text{(2.6a)} \qquad \frac{dx}{dt} = -\lambda_2 x + \alpha_2 \frac{xy}{1+x+y}(1-\gamma x),$$

$$\text{(2.6b)} \qquad \frac{dy}{dt} = \lambda_1 y - \alpha_1 \frac{xy}{1+x+y}.$$

Competition between the two populations can be effective only if $\alpha_1 > \lambda_1$, and $\alpha_2 > \lambda_1$, for if $\alpha_1 \le \lambda_1$, y could never decrease while if $\alpha_2 \le \lambda_2$, x could never increase. Therefore solutions will be sought for

$$\text{(2.7)} \qquad \alpha_1 > \lambda_1, \quad \alpha_2 > \lambda_2.$$

In the next sections the qualitative behaviour of solutions of (2.6a,b) will be studied and especially the dependence of the qualitative behaviour of solutions with respect to the parameters α_1, α_2, λ_1, λ_2 and γ. A special case is $\gamma = 0$, that is, $\theta = \infty$, which means that the antibody production is unlimited.

The solution of the differential equations (2.6a,b) will be discussed in the quarter plane

$$\mathbb{R}_+^2 = \{\binom{x}{y} \mid x > 0,\ y > 0\}.$$

On the boundary of this domain the solutions of (2.6a,b) satsify

$$\frac{dy}{dx} = 0 \quad \text{if} \quad y = 0, \quad \frac{dx}{dy} = 0 \quad \text{if} \quad x = 0.$$

It follows that no solution of (2.6a,b) with initial value in $\mathbb{R}^2_+$ can pass the lines $x = 0$, $y = 0$. Note that only $\mathbb{R}^2_+$ is of physical (biological) interest.

REMARK 2.8. In $\mathbb{R}^2_+$ the right-hand sides of (2.6a,b) satisfy the conditions for existence and uniqueness of solutions with initial values in $\mathbb{R}^2_+$. See HALE [4, chapter I, theorem 3.1].

3. MATHEMATICAL PRELIMINARIES

Throughout this chapter we will be concerned with the differential equation

$$\frac{d\xi}{dt} = F(\xi,\beta), \tag{3.1}$$

where $\xi = \begin{pmatrix} x \\ y \end{pmatrix}$, $F\colon \mathbb{R}_+^2 \times \mathbb{R} \to \mathbb{R}^2$ is given by the right-hand sides of (2.6a,b) and $\beta \in \mathbb{R}$ is composed of the parameters λ_1, λ_2, α_1, α_2 and γ. In chapter IV some features of equilibrium points of this type of differential equations were treated. The aim of the present chapter is to say something about periodic solutions of (3.1).

Let us recall that an equilibrium point ξ_0 is defined as a solution of the equation $F(\xi,\beta) = 0$, and that the stability of ξ_0, as a solution of (3.1), will be determined by the sign of the real parts of the eigenvalues of the Jacobian matrix $F'(\xi_0,\beta)$, the derivative of $F(\cdot,\beta)$ with respect to ξ at ξ_0. The equilibrium point ξ_0 and the eigenvalues are functions of the parameter β. Small changes in β may cause interesting modifications in the qualitative behaviour of solutions of (3.1).

The eigenvalues of $F'(\xi_0,\beta)$ are denoted by μ_1 and μ_2. Since F is real, μ_1 and μ_2 are both real or complex conjugated.

Let $\phi \in \mathbb{R}^2$ be a solution of (3.1). The *integral curve* of a solution $\phi(t)$ is the curve given by $\xi = \phi(t)$ in the ξ-space with t as a parameter. The direction of the curve is positive for increasing t. The behaviour of the integral curve of $\phi(t)$ in a neighbourhood of an equilibrium point ξ_0 depends on the derivative $F'(\xi_0,\beta)$, especially on the eigenvalues μ_1 and μ_2 of this linear mapping.

3.1. TYPES OF EQUILIBRIUM POINTS

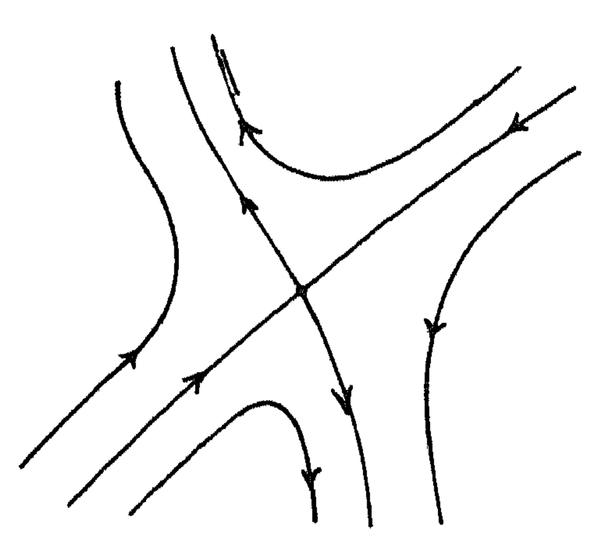
We make use of the following terminology for equilibrium points (figure 1 gives integral curves in a neighbourhood of an equilibrium point).

Case a. Both eigenvalues μ_1 and μ_2 are real and have opposite sign. Then the equilibrium point is called a *saddle point*. There are four exceptional curves: S_1 and S_3 going into ξ_0 and S_2 and S_4 going out of ξ_0. These curves are called *separatrices*. They will play an important role in section 6.

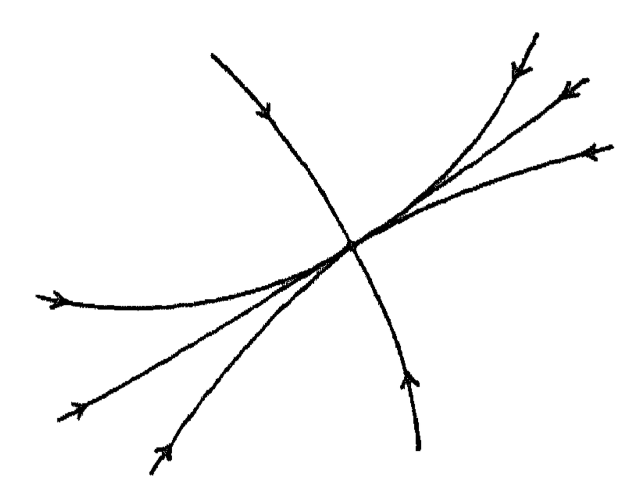
Case b. Both eigenvalues μ_1 and μ_2 are real and have the same sign. If $\mu_1 < 0$ (>0) then the equilibrium point is a stable (unstable) *node*.

Case c. $\mu_1 = \bar{\mu}_2$. If Re $\mu_1 < 0$ (>0) then the equilibrium point is a stable (unstable) *focus*. A solution spirals into (out of) ξ_0.

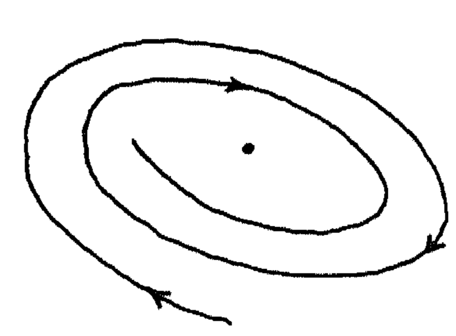
Case d. If there is a dense family of periodic solutions in a neighbourhood of the equilibrium point, then this point is called a *center*. A necessary condition for a center is $\mu_1 = \bar{\mu}_2$ and Re $\mu_1 = 0$. This condition is not sufficient. If $F(\xi,\beta)$ is nonlinear then the equilibrium point can be a focus or a center if Re $\mu_1 = 0$. In section 4 an example is given where ξ_0 is a center and in section 5 ξ_0 becomes a stable focus.



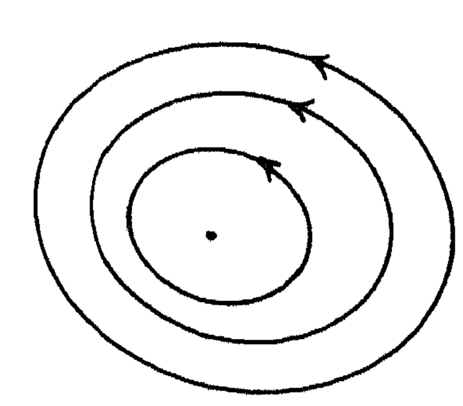
a. saddle point



b. stable node



c. stable focus



d. center

Figure 1

Note that if ξ_0 is an unstable equilibrium point then an integral curve approaches ξ_0 for $t \to -\infty$.

3.2. THE BIFURCATION THEOREMS OF FRIEDRICHS AND HOPF

To prove the existence of a branch of periodic solutions in the neighbourhood of an equilibrium point ξ_0 we make use of a bifurcation theorem of FRIEDRICHS [5]. This theorem is valid in a two-dimensional system. For reasons of completeness we also give a bifurcation theorem of HOPF [6], which is valid for higher dimensional systems and in addition gives information about the stability of the periodic solutions.

Let us write $\xi_0(\beta)$ for the equilibrium point as a function of β. Then $F(\xi_0(\beta),\beta) = 0$. As mentioned earlier, we are interested in the case that μ_1 and μ_2 cross the imaginary axis for some value of β. We suppose that this happens for $\beta = \beta_0$. In both of the following theorems a parameter $\varepsilon \in \mathbb{R}$ is necessarily introduced because of the non-analytic dependence of the family of periodic solutions on β at β_0. For the proofs of the theorems the reader is referred to the literature.

THEOREM 3.1. (FRIEDRICHS)
Suppose (3.1) *has an equilibrium point* $\xi_0(\beta)$ *such that* $F'(\xi_0(\beta_0),\beta_0)$ *has purely imaginary eigenvalues* $\pm\, i\omega_0$, $\omega_0 \neq 0$. *Suppose that the trace of the matrix*

$$\frac{d}{d\beta} F'(\xi_0(\beta),\beta) \tag{3.2}$$

does not vanish at β_0. *Then there exist functions* $\beta(\varepsilon)$ *and* $P(\varepsilon)$ *of an additional parameter* ε *such that* $\beta(0) = \beta_0$, $P(0) = P_0 = 2\pi/\omega_0$ *and* $d\beta/d\varepsilon = 0$, $dP/d\varepsilon = 0$ *at* $\varepsilon = 0$, *and further a function* $\eta(s,\varepsilon)$ *with period* P_0 *in* s, *assuming a prescribed value* $\eta(0,\varepsilon) = b_0$ *for* $s = 0$, *such that for sufficiently small values of* ε *the function*

$$\xi(t) = \xi_0(\beta(\varepsilon)) + \varepsilon\eta\left(\frac{P_0}{P(\varepsilon)}\, t,\varepsilon\right) \tag{3.3}$$

is a solution of the differential equation

$$\frac{d\xi}{dt} = F(\xi,\beta(\varepsilon)).$$

THEOREM 3.2. (HOPF)
Suppose (3.1), *with* $\xi \in \mathbb{R}^n$ *and* $F\colon \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$, *has an equilibrium point* $\xi_0(\beta)$ *such that* $F'(\xi_0(\beta_0),\beta_0)$ *has exactly two purely imaginary eigenvalues* $\mu_1(\beta_0) = i\omega_0$, $\mu_2(\beta_0) = -\, i\omega_0$, $\omega_0 \neq 0$. *Suppose further*

$$\mathrm{Re}\, \frac{d\mu_i(\beta)}{d\beta} \neq 0 \quad \text{at} \quad \beta = \beta_0,\ i = 1,2, \tag{3.4}$$

then there exists a function $\beta(\varepsilon)$, *with* $\beta(0) = \beta_0$ *and a set of real periodic solutions* $\xi = \xi(t,\varepsilon)$, $\xi(t,0) = \xi_0(\beta_0)$, *but* $\xi(t,\varepsilon) \neq \xi_0(\beta(\varepsilon))$ *for all sufficiently small* $\varepsilon \neq 0$; $\beta(\varepsilon)$ *and* $\xi(t,\varepsilon)$ *are analytic functions of* ε. *The* *same is true for the period* $P(\varepsilon)$ *of* $\xi(t,\varepsilon)$, *and* $P(0) = 2\pi/\omega_0$.

The periodic solutions exist with sufficiently small $\beta - \beta_0$ *either only for* $\beta > \beta_0$ *or only for* $\beta < \beta_0$ *(general case), or else only for* $\beta = \beta_0$. *If for* $\beta > \beta_0$ *all eigenvalues of the equilibrium point* $\xi_0(\beta)$ *have negative real parts (stability), then the following alternatives are valid in the general case. Either the periodic solutions branch from the equilibrium point after the latter has become unstable* $(\beta<\beta_0)$ *in which case the non-trivial periodic solutions are stable, or else the branching family of periodic solutions existed beforehand* $(\beta>\beta_0)$ *in which case these periodic solutions are unstable.*

REMARK 3.3. The branching at β_0 from a stable equilibrium point for $\beta > \beta_0$ to stable periodic solutions for $\beta < \beta_0$ is called supercritical branching, while the opposite case, where nontrivial periodic solutions pre-exist for $\beta > \beta_0$, is called subcritical branching (cf. section IV. 5.1).

REMARK 3.4. The second part of theorem 3.2 is the analogue of theorem IV.5.1. An equivalent theorem is proved by JOSEPH & SATTINGER [7] by means of perturbation theory.

3.3. SOME REMARKS ABOUT INTEGRAL CURVES IN THE PLANE AND THE THEOREM OF POINCARÉ-BENDIXSON

As noted in remark 2.8, in our case the uniqueness of a solution of (3.1) is guaranteed. An important corollary of the uniqueness of a solution of the autonomous system (3.1) is that integral curves cannot intersect each other.

In order to formulate the results in this subsection we introduce the following concepts. Some of these concepts and results are not restricted to the case of two dimensions. In these cases we suppose as in Hopf's theorem $\xi \in \mathbb{R}^n$, $F\colon \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$.

The *positive* or ω-*limit set* $\omega(\phi)$ of an integral curve $\xi = \phi(t)$ of (3.1) is the set of points which are approached along $\xi = \phi(t)$ with increasing time. More precisely, $q \in \omega(\phi)$, if there exists a sequence of real numbers $\{t_k\}$, $t_k \to \infty$ such that $\phi(t_k) \to q$ as $k \to \infty$. Similarly a point q belongs to the *negative limit set* or α-*limit set* $\alpha(\phi)$ if there is a sequence of real numbers $\{t_k\}$, $t_k \to -\infty$ as $k \to \infty$ such that $\phi(t_k) \to q$ as $k \to \infty$.

If $\phi(t)$ is an integral curve which appraoches to a periodic curve then that periodic curve is called the *limit cycle* of $\phi(t)$.

A set K in ξ-space is called an *invariant set* of (3.1) if, for any p in K with $\phi(t_0) = p$, the solution $\phi(t)$ of (3.1) belongs to K for t in $(-\infty,\infty)$. A set K is called *positively (negatively)* invariant if $\phi(t)$ belongs to K for $t \geq t_0$ $(\leq t_0)$.

Note that the integral curve of a periodic solution of (3.1) is an invariant set. The domain bounded by this integral curve is an invariant set too in the two-dimensional case.

The following theorem is given by HALE [4, chapter I, theorem 8.2.] and is proved there with Brouwer's fixed point theorem.

THEOREM 3.5. *If* K *is a positively invariant set of system* (3.1) *and* K *is homeomorphic to the closed unit ball in* $\mathbb{R}^n$, *then there is at least one equilibrium point of system* (3.1) *in* K.

The remaining items apply to the two-dimensional case.

COROLLARY 3.6. *The integral curve of a periodic solution of a two-dimensional system contains at least one equilibrium point in its interior.*

We conclude this section with some important theorems about the ω - (and α-) limit sets of an integral curve $\xi = \phi(t)$. (HALE [4, chapter II, theorem 1.2 and 1.3])

THEOREM 3.7. (POINCARÉ-BENDIXSON)
If $\xi = \phi(t) \in \mathbb{R}^2$ *is bounded for* $t > t_0$ *and the* ω*-limit set of* ϕ *does not contain an equilibrium point then either*
(i) $\dot{\phi}(t) = \omega(\phi)$
or
(ii) $\omega(\phi)$ *is the limit cycle of* ϕ.
In either case the ω*-limit set is a periodic orbit.*

THEOREM 3.8. *Let* ϕ *be an integral curve in a positively invariant subset* K *of* $\mathbb{R}^2$ *and suppose* K *has only a finite number of critical points. Then one of the following is satisfied:*
(i) $\omega(\phi)$ *is a critical point*
(ii) $\omega(\phi)$ *is a periodic orbit*
(iii) $\omega(\phi)$ *contains a finite number of critical points and a set of orbits* γ_i *with* $\alpha(\gamma_i)$ *and* $\omega(\gamma_i)$ *consisting of a critical point for each orbit* γ_i.

4. UNLIMITED ANTIBODY PRODUCTION (γ=0)

In this section we discuss the qualitative behaviour of the differential equations (2.6a,b) with $\gamma = 0$. In order to facilitate the investigation in the phase plane $\mathbb{R}_+^2$ we change variables from t to s by putting

$$s = \int_0^t \frac{d\tau}{1+x(\tau)+y(\tau)} \tag{4.1.}$$

from which we obtain the equivalent equations

$$\frac{d\xi}{ds} = F(\xi) \tag{4.2}$$

where

$$\xi = \begin{pmatrix} x \\ y \end{pmatrix}, \quad F(\xi) = \begin{pmatrix} x\{-\lambda_2-\lambda_2 x+(\alpha_2-\lambda_2)y\} \\ y\{\lambda_1-(\alpha_1-\lambda_1)x+\lambda_1 y\} \end{pmatrix}. \tag{4.3}$$

Assuming that we can solve (4.2) for x(s) and y(s), it is then possible to obtain solutions of (2.6a,b) in terms of the original independent variable

$$t = \int_0^s \{1 + x(\sigma) + y(\sigma)\}\, d\sigma.$$

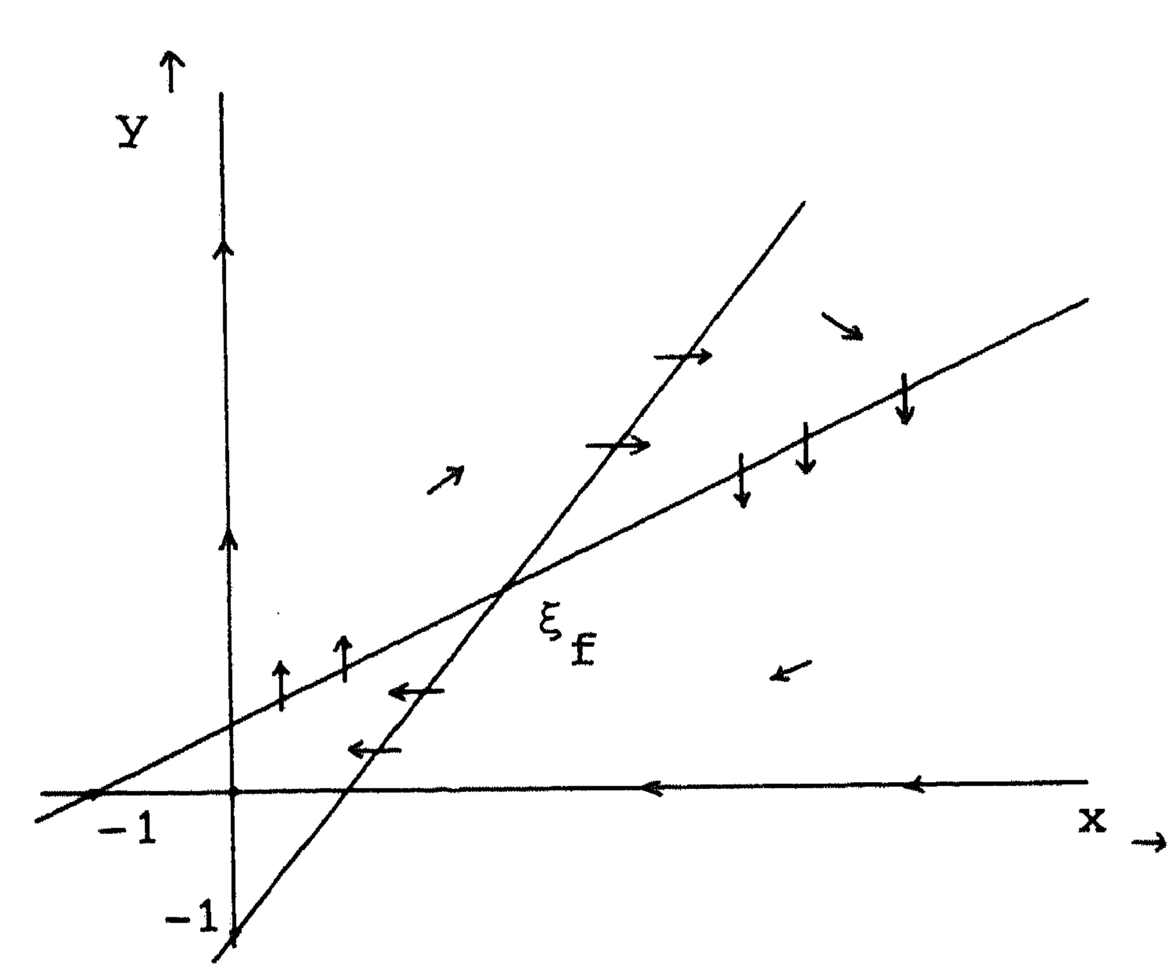


Figure 2

A phase plane investigation is useful in discussing (4.2), see figure 2. The equilibrium points are $\xi = 0$ and $\xi = \xi_f$, where the latter point is the point of intersection of the two lines

$$(4.4) \qquad y = \frac{\lambda_2}{\alpha_2-\lambda_2}(1+x), \qquad y = \frac{\alpha_1-\lambda_1}{\lambda_1}x - 1.$$

The origin is a saddle point with the vertical axis ($y\geq 0, x=0$) as an outwardly directed separatrix ($dy/ds>0$, $dx/ds=0$) and the horizontal axis ($y=0, x\geq 0$) as an inwardly directed separatrix ($dx/ds<0$, $dy/ds=0$).

Let us introduce the quantity

$$(4.5) \qquad R = \alpha_1\alpha_2 - \alpha_1\lambda_2 - \alpha_2\lambda_1,$$

then

$$(4.6) \qquad \xi_f = \begin{pmatrix} x_f \\ y_f \end{pmatrix} = \begin{pmatrix} \alpha_2\lambda_1/R \\ \alpha_1\lambda_2/R \end{pmatrix}, \qquad R \neq 0.$$

Hence, the lines (4.4) will intersect in $\mathbb{R}^2_+$ if and only if $R > 0$. If $R \leq 0$, the direction field is as in figure 3. All integral curves tend towards $x = \infty$, $y = \infty$. In this case the response is not sufficient to terminate the proliferation of antigen.

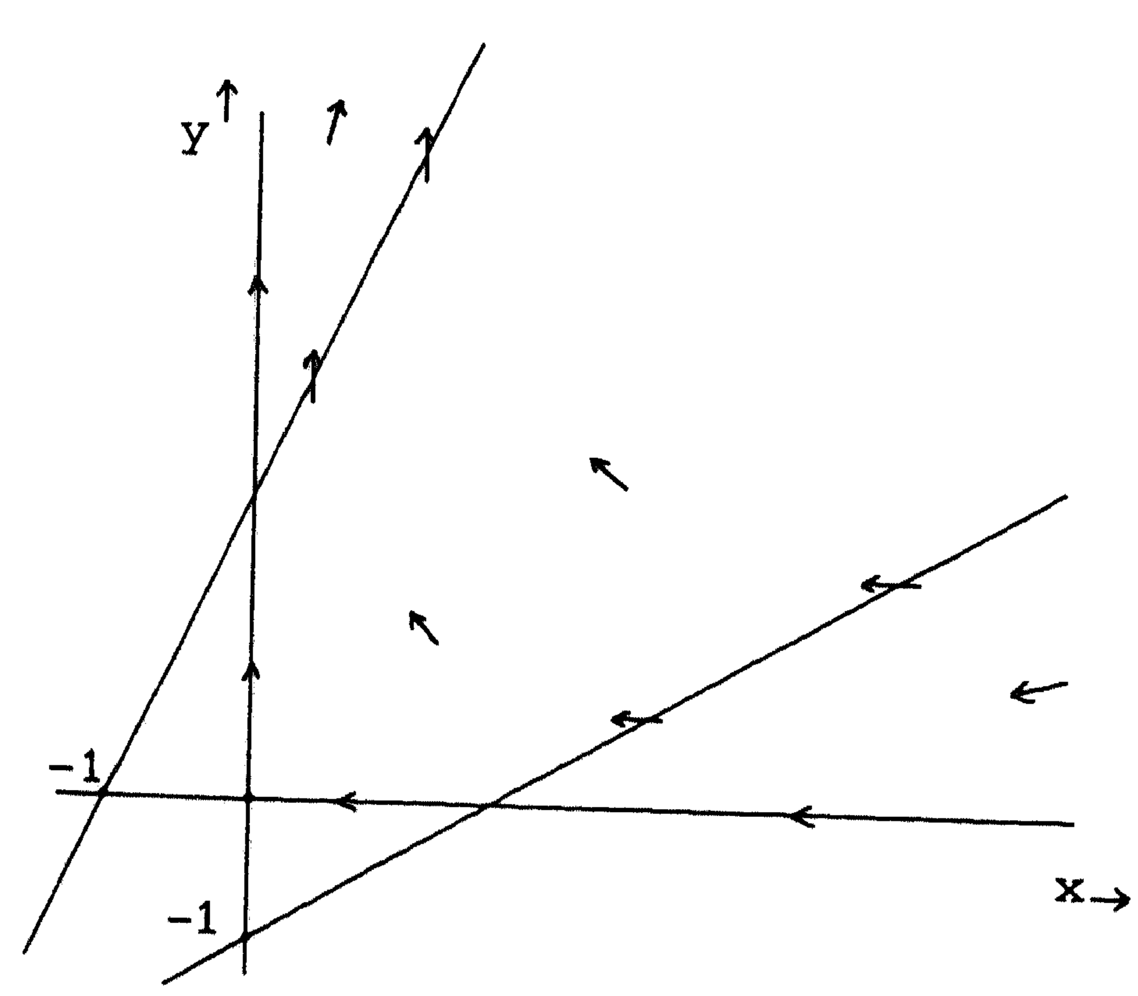


Figure 3

We are interested in periodic solutions of (4.2). If $R \leq 0$ no periodic solutions will occur. So, henceforth we assume $R > 0$. Moreover we suppose that (2.7) holds.

The stability character of the equilibrium point ξ_f depends on the eigenvalues of $F'(\xi_f)$, this matrix being given by

$$(4.7) \qquad F'(\xi_f) = \begin{pmatrix} -\lambda_2 x_f & (\alpha_2-\lambda_2)x_f \\ -(\alpha_1-\lambda_1)y_f & \lambda_1 y_f \end{pmatrix}.$$

The eigenvalues of this matrix μ_1 and μ_2 are the solutions of

$$(4.8) \qquad \mu^2 + \frac{\lambda_1\lambda_2(\alpha_2-\alpha_1)}{R}\mu + \frac{\alpha_1\alpha_2\lambda_1\lambda_2}{R} = 0.$$

For periodic solutions μ_1 and μ_2 have to be complex conjugated and so we assume that the discriminant of (4.8) is negative, yielding

$$(4.9) \qquad R > \frac{(\alpha_1-\alpha_2)^2\lambda_1\lambda_2}{4\alpha_1\alpha_2}.$$

Because of $\mu_1 = \bar{\mu}_2$

$$(4.10) \qquad \operatorname{Re} \mu_i = -\frac{\lambda_1\lambda_2(\alpha_2-\alpha_1)}{2R}$$

and thus ξ_f is a focal point towards which the solutions converge if $\alpha_1 < \alpha_2$ and from which they emanate if $\alpha_1 > \alpha_2$.

If (4.9) is not satisfied, the two eigenvalues μ_i are real and of the same sign. The point ξ_f is a node to which the solutions converge if $\alpha_1 > \alpha_2$ and from which they emerge if $\alpha_1 > \alpha_2$. Thus, irrespective of whether ξ_f is a node or a focal point, it is attracting solutions if $\alpha_2 > \alpha_1$ and repelling solutions if $\alpha_1 > \alpha_2$. In both cases, $\operatorname{ind}(F,\xi_f,0) = 1$.

It will be shown that if

$$(4.11) \qquad \alpha_1 = \alpha_2 \quad (=\alpha),$$

(4.2) has a set of periodic solutions around ξ_f. Note that for (4.11) the condition $R > 0$ becomes

$$(4.12) \qquad \alpha > \lambda_1 + \lambda_2.$$

In the case of (4.11) the solution of (4.2) can be explicitly found. It is given by

$$C(1+x+y)^{\alpha} = x^{\lambda_1} y^{\lambda_2}, \tag{4.13}$$

where C is a constant of integration.

LEMMA 4.1. *Let* (4.11) *and* (4.12) *be satisified. Then* (4.2) *has a set of periodic solutions around* ξ_f.

PROOF. Consider the scalar function $z\colon \mathbb{R}^2 \to \mathbb{R}$ given by (see (4.13))

$$z = x^{\lambda_1} y^{\lambda_2}(1+x+y)^{-\alpha}.$$

Then $z(0,y) = z(x,0) = 0$ and, owing to (4.12), $z \to 0$ if x and/or y tend to infinity; z has an absolute maximum in ξ_f and hence the equation $z(x,y) = C$ defines a periodic solution for all C satisfying

$$0 \le C \le z(x_f, y_f).$$

This proves the lemma. □

So we can describe the bifurcation phenomenon in the neighbourhood of ξ_f in terms of the parameter α_1, with α_2, λ_1, λ_2, (γ=0) fixed, as follows. Starting with a value of $\alpha_1 < \alpha_2$ all solutions starting in a certain neighbourhood of ξ_f will go into ξ_f, and ξ_f is stable solution.

If $\alpha_1 = \alpha_2$ then a family of periodic solutions occurs in a neighbourhood of ξ_f. This is a case of vertical bifurcation (see figure 4).

If $\alpha_1 > \alpha_2$ then any solution starting in a certain neighbourhood of ξ_f will leave this neighbourhood and ξ_f is an unstable equilibrium point.

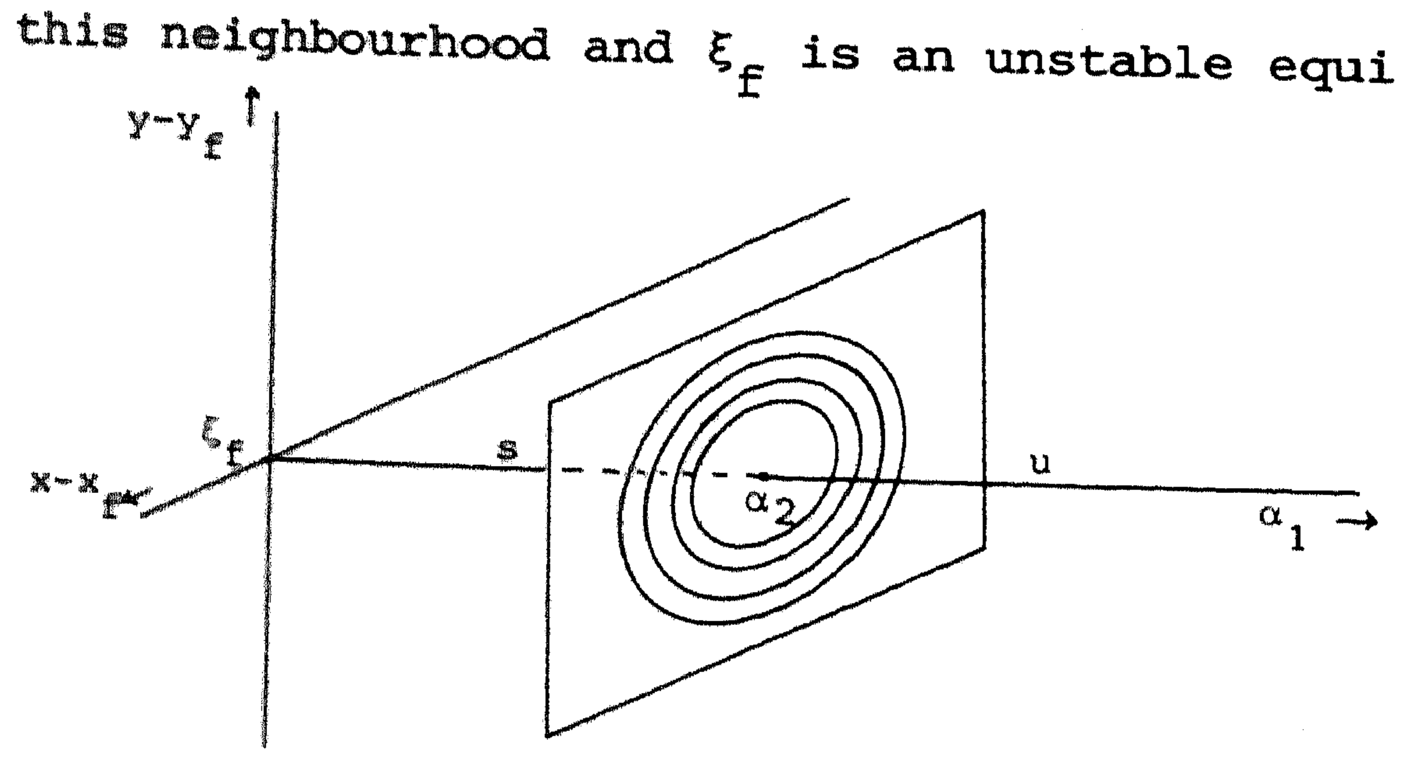


Figure 4

5. LIMITED ANTIBODY PRODUCTION ($\gamma \neq 0$)

In the preceding section equations (2.6a,b) were considered with $\gamma = 0$, that is, with no limits placed on the amount of antibody that can be produced. In this section, the antibody production will be limited, by choosing $\gamma > 0$, by a value $A_b = x/k \le 1/(\gamma k)$. With $\gamma \neq 0$ we have after using the transformation (4.1).

$$\frac{d\xi}{ds} = F(\xi), \tag{5.1}$$

where

$$\xi = \begin{pmatrix} x \\ y \end{pmatrix}, \quad F(\xi) = \begin{pmatrix} f_1(x,y) \\ f_2(x,y) \end{pmatrix} = \begin{pmatrix} x\{-\lambda_2(1+x+y)+\alpha_2 y(1-\gamma x)\} \\ y\{\lambda_1-(\alpha_1-\lambda_1)x+\lambda_1 y\} \end{pmatrix} \tag{5.2}$$

Note that f_2 equals the corresponding component in (4.3). The equilibrium points of (5.1) are 0, ξ_f and ξ_s where the latter points are the intersections of (see figure 5)

$$y = \frac{\lambda_2(1+x)}{(\alpha_2-\lambda_2-\alpha_2\gamma x)} \quad \text{and} \quad y = \frac{\alpha_1-\lambda_1}{\lambda_1} x - 1. \tag{5.3}$$

In this section we make the assumptions (cf. (2.7) and (4.12))

$$\alpha_1 > \lambda_1, \ \alpha_2 > \lambda_2, \ \alpha_1 > \lambda_1 + \lambda_2, \ \alpha_2 > \lambda_1 + \lambda_2. \tag{5.4}$$

The first of (5.3) describes a curve with a vertical asymptote at $x = x_a = (\alpha_2-\lambda_2)/(\alpha_2\gamma)$. If one starts from $0 \le x < x_a$ and $y \ge 0$, it is impossible to reach values of $x \ge x_a$.

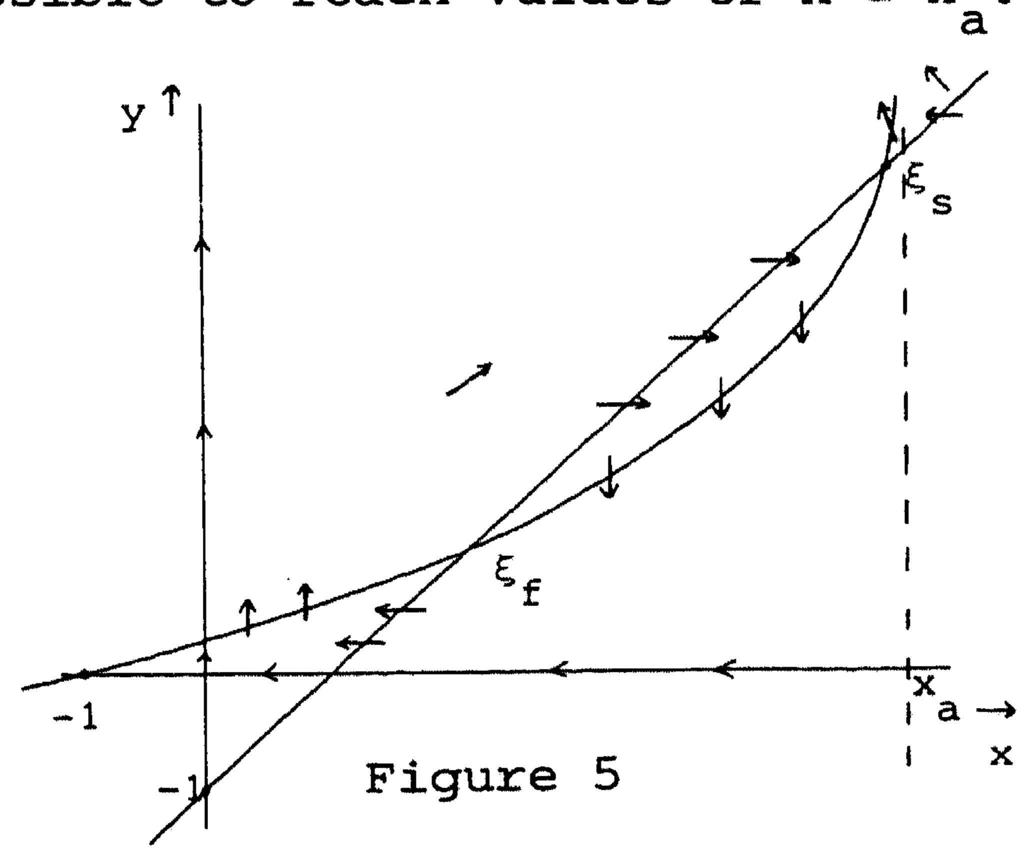


Figure 5

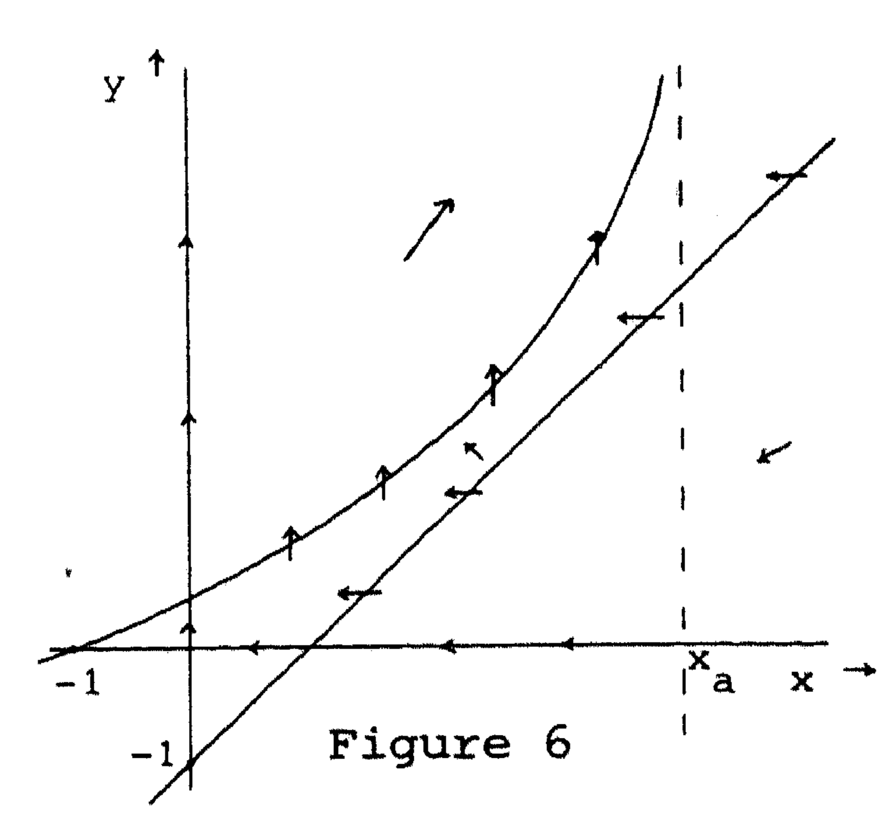


Figure 6

The curves given by (5.3) may or may not intersect for x in the range $0 \le x \le x_a$. If they do not, the trajectories will be as in figure 6. There will be unlimited antigen proliferation, and as $t \to \infty$ then $x \to x_a$ and $y \to \infty$.

In this section we are interested in periodic solutions of (5.1), which can only occur if the curves in (5.3) intersect twice because there must be an equilibrium point in the interior of their integral curve (cf. corollary 3.6). Clearly for $\gamma > 0$ and $\alpha_2 > \lambda_1 + \lambda_2$ fixed, α_1 can be taken large enough to make the curves in (5.3) intersect. In the following we assume that two intersections ξ_f and ξ_s exist as in figure 5.

Then (5.1) defines a direction field that can be traced in the phase plane as shown by the arrows. From figure 5 ξ_f is easily seen to be a focus, center or node, while 0 and ξ_s are saddle points. The same can be shown by considering $F'(\xi_s)$ and $F'(\xi_f)$.

In section 4 it was possible to take one of the model parameters (α_1 or α_2) as bifurcation parameter because of the simple expression for ξ_f in terms of the parameters. In this section the mathematics involved in the bifurcation phenomena become easier if we introduce an additional bifurcation parameter β in the following way.

(5.5) $$\frac{d\xi}{ds} = F(\xi,\beta)$$

where $F: \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}^2$ is given by

(5.6) $$F(\xi,\beta) = \begin{pmatrix} \beta f_1(x,y) \\ f_2(x,y) \end{pmatrix}$$

and f_1 and f_2 are given in (5.2).

An advantage of introducing the parameter β in this way is that the equilibrium points remain fixed when β is varied.

The model given by (5.5) with $\beta = 1$ is the same as our original model (5.1). We will show that periodic solutions in the neighbourhood of some critical value β_0 will exist and moreover that periodic solutions will occur in model (5.1). The value β_0 is a function of α_1, α_2, λ_1, λ_2 and γ and can pass the value $\beta_0 = 1$ by varying some of these parameters.

Form the character of the equilibrium points it follows that periodic solutions can only branch from

$$\xi_f = \begin{pmatrix} x_f \\ y_f \end{pmatrix}$$

Computing the derivative of $F(.,\beta)$ with respect to ξ at ξ_f yields

$$F'(\xi_f,\beta) = \begin{pmatrix} -\beta\lambda_2 x_f - \beta\alpha_2\gamma x_f y_f & -\beta\lambda_2 x_f + \beta\alpha_2(1-\gamma x_f) \\ -(\alpha_1-\lambda_1)y_f & \lambda_1 y_f \end{pmatrix}. \tag{5.7}$$

The eigenvalues μ_1 and μ_2 are the solutions of the equation

$$\mu^2 + b\mu + \beta x_f y_f c = 0, \tag{5.8}$$

where

$$b = -\lambda_1 y_f + \beta\lambda_2 x_f + \beta\alpha_2\gamma x_f y_f ,$$

$$c = -\lambda_1(\lambda_2+\alpha_2\gamma y_f) + (\alpha_1-\lambda_1)(\alpha_2-\lambda_2-\alpha_2\gamma x_f)$$

and c can be shown to be positive.

Hence the eigenvalues μ_1 and μ_2 are purely imaginary if $b = 0$. This yields the bifurcation point

$$\beta_0 = \frac{\lambda_1 y_f}{\lambda_2 x_f + \alpha_2\gamma x_f y_f} . \tag{5.9}$$

For β in the neighbourhood of β_0 the eigenvalues are complex conjugated.

In order to apply Friedrichs' bifurcation theorem (theorem 3.1) we still have to check if the trace of

$$\frac{d}{d\beta} F'(\xi_f(\beta), \beta)\big|_{\beta=\beta_0} = \begin{pmatrix} -\lambda_2 x_f - \alpha_2\gamma x_f y_f & -\lambda_2 x_f + \alpha_2(1-\gamma x_f) \\ 0 & 0 \end{pmatrix} \tag{5.10}$$

does not vanish. (Note that ξ_f does not depend on β.) On inspection this condition is satisfied.

Accordingly, there does indeed exist a continuous one-parameter family of periodic solutions of (5.5) branching at β_0 from ξ_f in the case $\gamma > 0$, assuming that the curves in (5.3) intersect as in figure 5, as was asserted.

By the theorem of HOPF (theorem 3.2) our family of periodic solutions is unique in a neighbourhood of ξ_f and exists on one side of β_0 only (if the bifurcation is not vertical). If $\beta > \beta_0$ then $b > 0$ and $\mathrm{Re}\,\mu_1 = \mathrm{Re}\,\mu_2 < 0$ and so ξ_f is stable. If $\beta < \beta_0$ the equilibrium point ξ_f is unstable.

There are two possibilities: supercritical and subcritical branching (see figures 7 and 8 respectively) and we will make clear which of the cases applies.

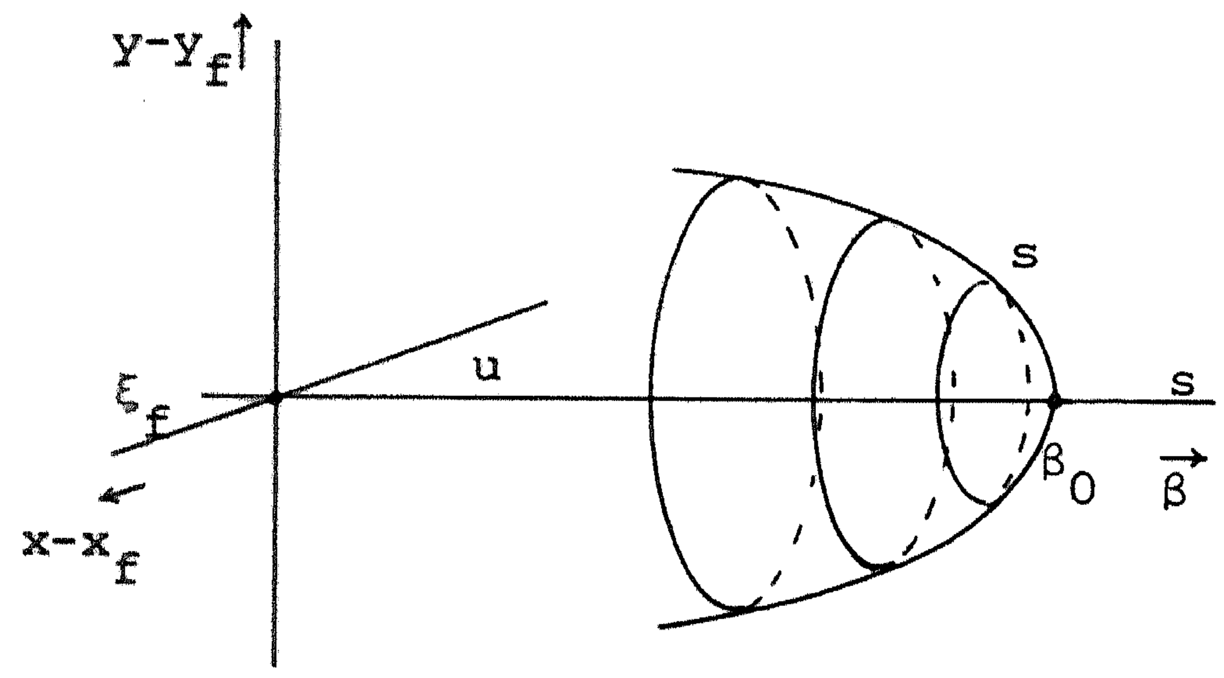


Figure 7

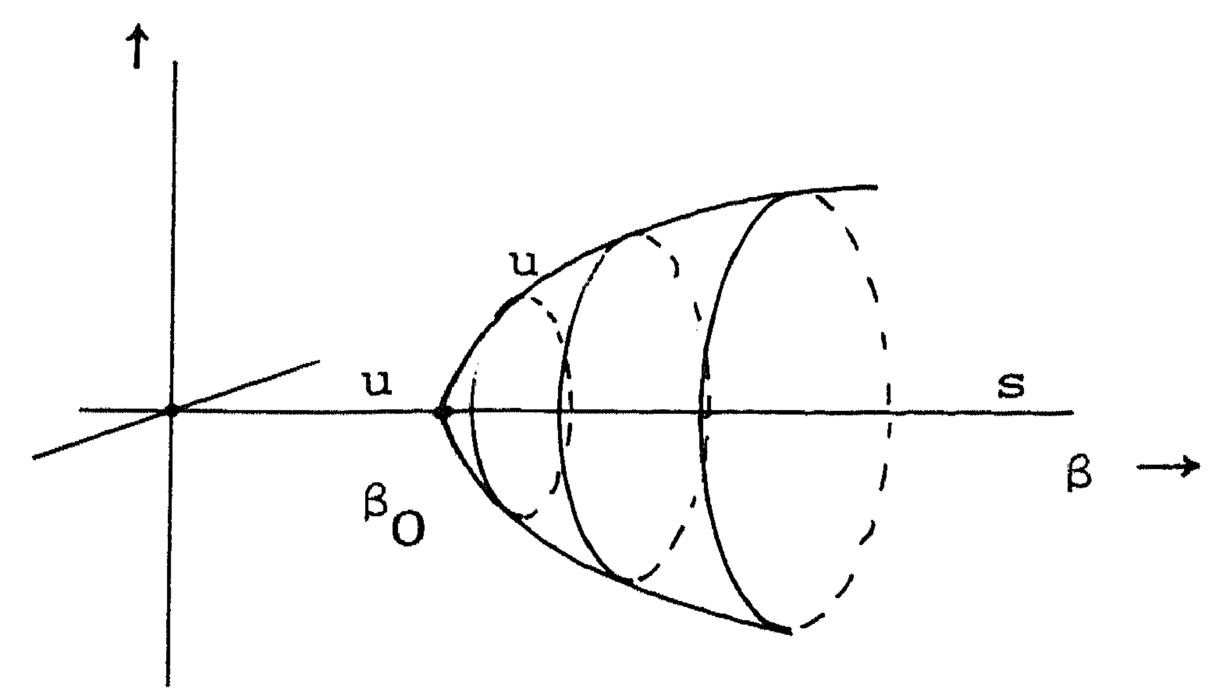


Figure 8

PIMBLEY [3] proofs that ξ_f is stable at $\beta = \beta_0$. His proof involves many calculations and will not be given here.

Because of the stability of ξ_f at $\beta = \beta_0$ subcritical branching is impossible. Namely, in the case of subcritical branching the periodic solutions will be unstable and that would imply a discontinuity in the direction field of (5.5) at $\beta = \beta_0$ since we should then pass from unstable periodic solutions for $\beta > \beta_0$ through a stable constant solution at β_0, and then to an unstable constant solution ξ_f for $\beta < \beta_0$, as β is decreased through β_0. This discontinuity cannot exist at β_0 since the right-hand sides of (5.5) are continuous in β, x, y. Thus we have supercritical branching of stable periodic solutions at β_0 if ξ_f is stable at β_0.

The usual technique to determine on which side of the critical value β_0 the bifurcated periodic solutions of equations like (5.5) are situated is by means of the perturbation series for (5.5) (cf. PIMBLEY [2, (16)], SATTINGER [6]. We write

$$\begin{aligned} x &= x_f + \varepsilon x_0 + \varepsilon^2 x_1 + \varepsilon^3 x_2 + \dots \\ y &= y_f + \varepsilon y_0 + \varepsilon^2 y_1 + \varepsilon^3 y_2 + \dots \\ \beta &= \beta_0 + \varepsilon\beta + \varepsilon^2\beta_2 + \dots \\ P &= P_0 + \varepsilon P_1 + \varepsilon^2 P_2 + \dots \end{aligned} \tag{5.11}$$

and substitute $\eta = \frac{P_0}{P(\varepsilon)} s$ into (5.5) as a new independent variable. Here ε is the additional parameter mentioned in Friedrichs' theorem 3.1. By Friedrichs' theorem $\beta_1 = \beta_\varepsilon(0) = 0$ and $P_1 = P_\varepsilon(0) = 0$, and the functions $\beta(\varepsilon)$ and $P(\varepsilon)$ can be assumed to be analytic. Thus expansions (5.11) converge in some neighbourhood of $\varepsilon = 0$. If $\beta_2 < 0$, bifurcation would occur for $\beta < \beta_0$, i.e., supercritical in our case. On the other hand, if $\beta_2 > 0$ the bifurcation will be for $\beta > \beta_0$, i.e., subcritical.

The constants β_2 and P_2 are found from the hierarchy equations for (x_2, y_2), solved with the conditions $x_2(0) = x_2(P_0) = 0$, $y_2(0) = y_2(P_0) = 0$. To cite Pimbley:
"Very lengthy expressions result for β_2 and P_2 which afford no visual insight regarding the sign of β_2".

Now we have seen that equation (5.5) yields periodic solutions for $\beta < \beta_0$ where β_0 is given by (5.9) as a function of the model parameters α_1, α_2, λ_1, λ_2 and γ; x_f and y_f are functions of α_1, α_2, λ_1, λ_2 and γ too.

For $\beta > \beta_0$ the equilibrium point is stable and in some neighbourhood of β_0 there are periodic solutions for $\beta < \beta_0$.

Our original model (5.1) corresponds with model (5.5) with $\beta = 1$. Thus for $\beta_0 < 1$, ξ_f is stable and there will occur periodic solutions if α_1, α_2, λ_1, λ_2, γ are varied such that $\beta_0 > 1$.

Let us consider the inequalities $\beta_0 \lesseqgtr 1$. From (5.9), these inequalities correspond with

$$\lambda_2 x_f + \alpha_2 \gamma x_f y_f - \lambda_1 y_f \lesseqgtr 0.$$

Now we can proof

<u>LEMMA 5.1</u>. *There exists a value $\alpha_1 = \alpha_{10} > \alpha_2$ such that $\beta_0 < 1$ if $\alpha_1 < \alpha_{10}$ and $\beta_0 > 1$ if $\alpha_1 > \alpha_{10}$.*

PROOF. Consider

$$(5.12)\qquad f(\alpha_1) = \lambda_2 x_f + \alpha_2\gamma x_f y_f - \lambda_1 y_f.$$

Substituting $\alpha_2 y_f \gamma x_f$ by means of the first of (5.3) yields

$$(5.13)\qquad f(\alpha_1) = -\lambda_2 + (\alpha_2-\lambda_2-\lambda_1)y_f$$

By inspection of figure 9, increasing α_1 results in decreasing x_f and y_f.

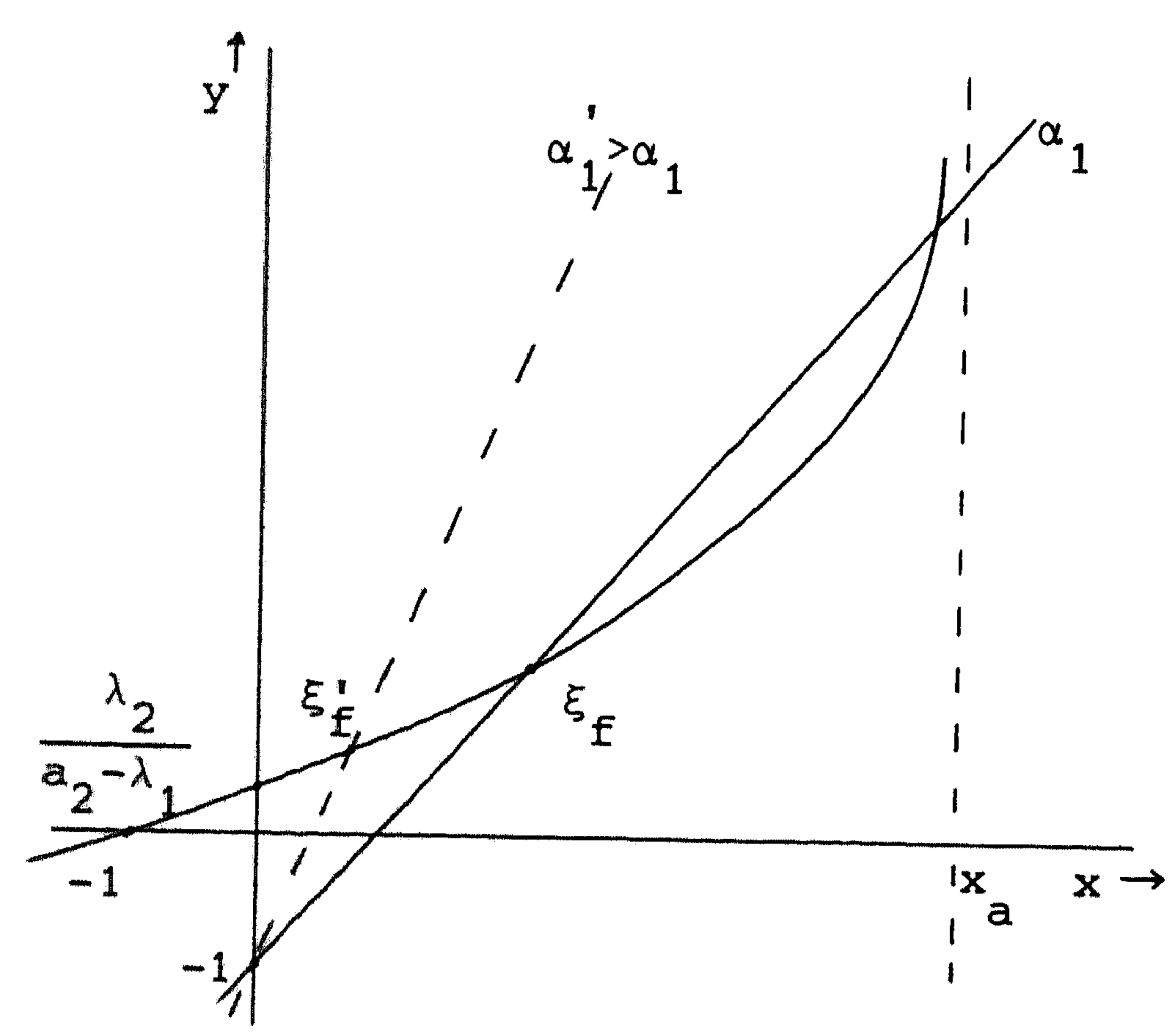


Figure 9

So $f(\alpha_1)$ is a nonincreasing function of α_1 (keeping $\alpha_2,\lambda_1,\lambda_2,\gamma$ fixed). Equations (5.3) yield

$$(5.14)\qquad \lambda_1[\lambda_2(1+x_f+y_f) - \alpha_2 y_f(1-\gamma x_f)] + \lambda_2[-\lambda_1+(\alpha_1-\lambda_1)x_f+\lambda_1 y_f] = 0.$$

If $\alpha_1 = \alpha_2$, (5.14) results in

$$(5.15)\qquad \lambda_1\gamma x_f y_f + \lambda_2 x_f - \lambda_1 y_f = 0.$$

From (5.15), (5.12) and (5.4)

$$(5.16)\qquad f(\alpha_2) > 0.$$

If $\alpha_1 \to \infty$, then $x_f \to 0$, $y_f \to \frac{\lambda_2}{\alpha_2-\lambda_2}$ and so

$$f(\alpha_1) \to -\lambda_2 + \frac{(\alpha_2-\lambda_2-\lambda_1)\lambda_2}{(\alpha_2-\lambda_2)} = -\frac{\lambda_1\lambda_2}{(\alpha_2-\lambda_2)} < 0$$

So the behaviour of $f(\alpha_1)$ will be as in figure 10.

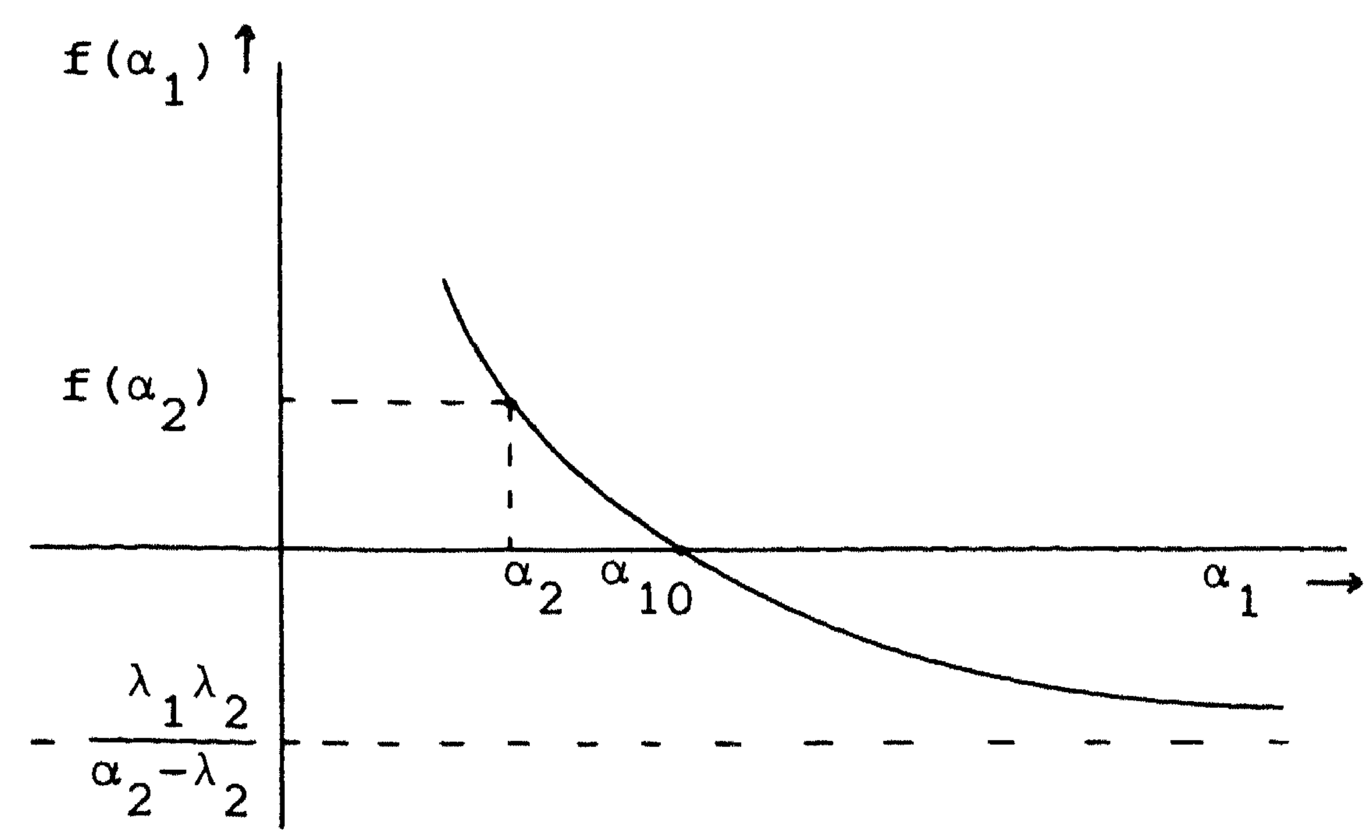


Figure 10

Thus there exists a critical value α_{10} such that $f(\alpha_{10}) = 0$, $f(\alpha_1) > 0$ if $\alpha_1 < \alpha_{10}$ and $f(\alpha_1) < 0$ if $\alpha_1 > \alpha_{10}$. The correspondence of $f(\alpha_1) \gtrless 0$ with $\beta_0 \lessgtr 1$ completes the proof. □

COROLLARY 5.2. *For α_2, λ_1, λ_2, γ fixed, there exists a value α_{10} such that the equilibrium point ξ_f is stable for $\alpha_1 \le \alpha_{10}$. There will occur stable periodic solutions in a neighbourhood of α_{10} for $\alpha_1 > \alpha_{10}$.*

6. SOME REMARKS ABOUT THE EXISTENCE OF PERIODIC SOLUTIONS

In sections 4 and 5 we have seen a family of periodic solutions branching from an equilibrium point ξ_f. The following question arises readily: have the models (4.2) and (5.1) more than one family of periodic solutions?

BELL [1] expects no other periodic solutions of (4.2) than those found in section 4, and his hypothesis is strengthened by numerical experiments. However, he is not able to prove that there are no other periodic solutions.

PIMBLEY [3] shows that for some value of $\beta = \beta^* < \beta_0$ the separatrices S_1 and S_2 in figure 11 will join to form a closed separatrix as in figure 12.

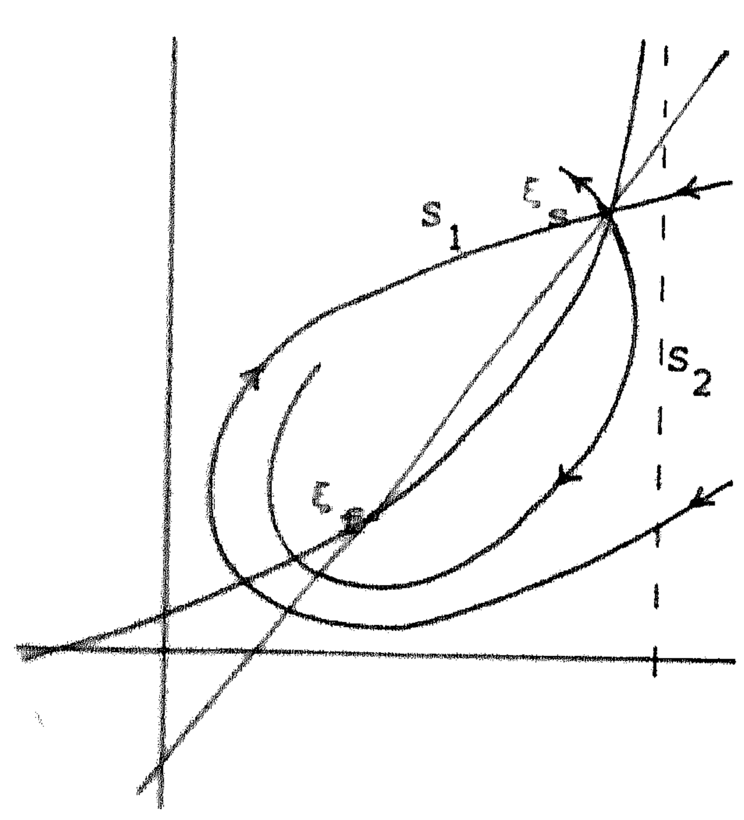


Figure 11

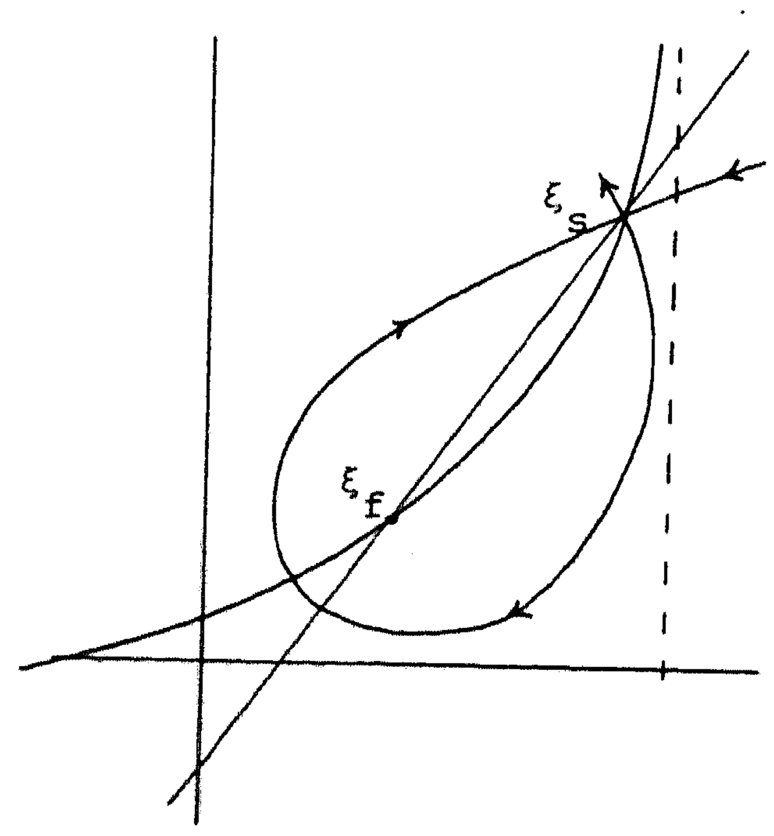


Figure 12

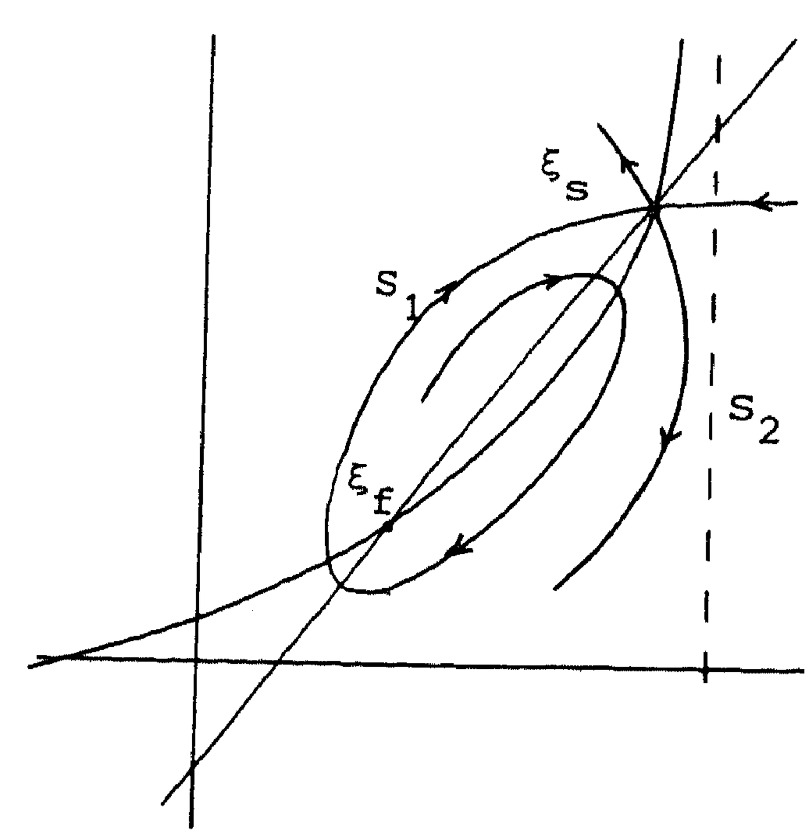


Figure 13

Using a result of ANDRONOV [9, p.299] he proves the existence of a family of periodic solutions branching from this closed separatrix. So his branching diagram becomes as in figure 14.

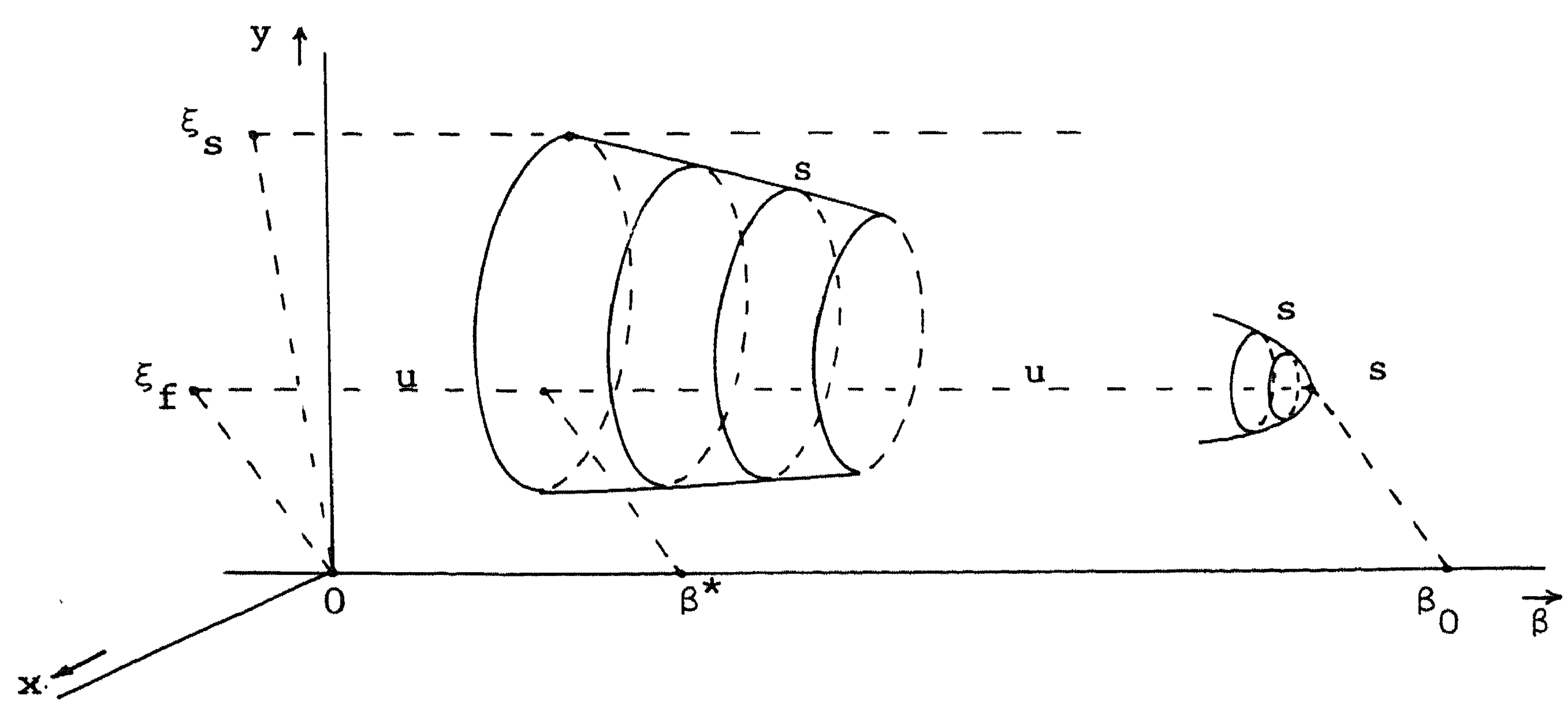


Figure 14

He thus has two continuous one-parameter families of periodic solutions for (5.5). One bifurcates from the equilibrium point ξ_f at β_0. The other one bifurcates from a closed separatrix at β^*. The amplitudes of the periodic solutions with values of β in a neighbourhood of β_0 are smaller than those of the periodic solutions in a neighbourhood of β^*.

A family of periodic solutions can be extended to a maximal family. If no secondary bifurcation occurs this family terminates either in an equilibrium point, or in a closed curve which contains at least one equilibrium point. In our case such a curve has to be a closed separatrix. If the family branching from ξ_f at β_0 can be extended to the closed separatrix at β^* then both families are identical.

Results concerning bifurcation from periodic solutions and closed separatrices can be found in ANDRONOV [9]. The qualitative aspects of bifurcation from periodic solutions are similar to those obtained in chapter IV, especially with respect to the (un)stability of the original and the bifurcated periodic solutions.

In search of periodic solutions of a differential equation we can make some remarks. Generally, a periodic solution can be found as a limit cycle of a solution. From the theorem of Poincaré-Bendixson (theorem 3.7) we know that if we can find a ring-like region in $\mathbb{R}^2$, free from equilibrium points, and if the vector field F is never directed outwardly (inwardly) on the boundary of the region, we can say that there exists at least one stable (unstable) limit-cycle (= periodic solution) within that region.

In the case of section 5 the separatrices S_1 and S_2 can be used for dividing the plane. If they do not join to form a closed separatrix, there are two possibilities: when the separatrix S_1 is followed backwards from ξ_s, either it will cross the vertical line $x = x_a$ and continue to still larger x (cf. figure 11), or it will spiral around or into ξ_f (figure 13). If in the case of figure 11 ξ_f is an unstable equilibrium point then at least one stable limit-cycle exists. If in the case of figure 13 ξ_f is a stable equilibrium point then there will be an unstable limit-cycle.

Finally we give a sufficient condition that no limit-cycles can exist.

THEOREM 6.1. (BENDIXSON'*s criterion*)
If

$$\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} \tag{6.1}$$

has a fixed sign, then there are no limit-cycles, and even no simple closed curve γ *made up of paths.*

PROOF. The proof is immediate. Suppose a closed integral curve γ exists which is a solution of

$$\frac{dx}{dt} = f_1, \qquad \frac{dy}{dt} = f_2. \tag{6.2}$$

By the theorem of Gauss, if D is the region bounded by γ, then

$$\iint_D \left(\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y}\right) dxdy = \oint_\gamma (f_1dy - f_2dx). \tag{6.3}$$

The left-hand side is $\neq 0$ on account of the fixed sign of the integrand, the right-hand side vanishes on account of the differential equation (6.2). This contradiction proves the theorem. □

This theorem gives some information on the position of a limit-cycle, if it exists. In the region D, bounded by the limit-cycle,

$$\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y}$$

has to change sign.

7. DISCUSSION

It has been seen that the equations for the struggle between antigen and antibody populations admit a rich variety of solutions depending on the model parameters, and it is tempting to compare such solutions with real immune responses. In view of the simplified nature of the model such comparisons should be taken lightly.

From a biological point of view we are interested in solutions such that the concentration of antigen remains bounded. In both models (4.2) and (5.2) we have seen that in a neighboorhood of ξ_f the solutions spiral into or away from ξ_f. This means that $x(= kA_b)$ and $y(= kA_g)$ oscillate in a neighboorhood of x_f and y_f. These oscillations can be damped (if ξ_f is stable) or they can be of increasing amplitude (if ξ_f is unstable).

In the model of section 4 we have seen that if α_1, the rate of bound antigen eliminating, is greater than α_2, the rate of antibody production, then there is a tendency for the oscillations to be of increasing amplitude. During such oscillations, it is possible for the antigen to be eliminated during an antigen minimum or for the host to be killed during antigen maximum. If on the other hand $\alpha_1 < \alpha_2$, the oscillations will be damped and a steady state will be reached in which antigen is present.

In the model of section 5 there is the possibility of a limit cycle which means that x and y have as a limit case oscillations with a fixed amplitude. From a biological point of view this model is more realistic than the one of section 4. First, since a limit on the antibody is natural. In the second place, since for $\alpha_1 = \alpha_2$ in the model of section 4 ξ_f will be a center. In this case, the qualitative behaviour of the solutions completely changes when the model is subjected to small perturbations. In section 5 stable limit cycles occur. This structure of solutions admits small perturbations of the model in the sense that the qualitative behaviour of the solutions will not change (cf. HALE [4, chapter V]; ANDRONOV [9] introduces the term structural stability for systems that admit small perturbations of the right-hand side of the differential equation).

Finally we make some remarks about a three-dimensional model recently investigated by PIMBLEY [10]. This model differs from the previous models in having a third population consisting of cells which produce antibodies when stimulated by antigen, and therefore leads to a system of three ordinary differential equations. This third order model is proposed as a biogically more realistic mathematical description of the process of the immune response than were the second order models. Indeed we know experimentally that antibody is produced by cells which have been stimulated to do so by antigen. Again an auxiliar parameter β is introduced and, using Hopf's theorem, Pimbley proves the existence of a family of periodic solutions branching from an equilibrium point ξ_f at β_0. With the third order model it is most difficult to find values of the parameters such that β_0 can be passed through unity and the direction of bifurcation, supercritical or subcritical, is quite equivocal indeed.

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