5

Numerical Methods for Dynamical Systems

Wolf-Jürgen Beyn

These lectures are intended to give a survey of numerical methods for analyzing dynamical systems. The growing interest in these systems, in particular in their chaotic behaviour, has stimulated an immense amount of theoretical as well as numerical investigation. Therefore we restrict ourselves to a few typical phenomena which are only first steps to chaos, but whose numerical properties are fairly well understood. Among the topics covered are the numerical computation of invariant sets such as stationary points, periodic orbits and tori, the transitions between these objects in parametrized systems and the analysis of the longtime behaviour of numerical trajectories which are generated with sufficiently small step-size.In particular, we discuss in some detail the numerical computation of singular points and of homoclinic orbits via defining equations.

5.1 Basic phenomena and numerical problems

In this chapter we discuss some basic notions and results from dynamical systems theory. These will help us in motivating the numerical questions relevant in this context. Since there is a vast literature on the subject, we do not attempt to give complete references, but rather follow our personal view. In many cases the references cited may be taken as a starting point for further study.

As some general references for the numerical part we quote here the monographs by Kubiček and Marek[63], Rheinboldt[80], Seydel[87] and the special volumes Küpper, Mittelmann and Weber[65], Küpper, Seydel and Troger[66] and J. of Comp. Appl. Math. 26 (1989).

5.1.1 Dynamical systems

We consider the time dependence of a system which can be described by an N-dimensional state vector

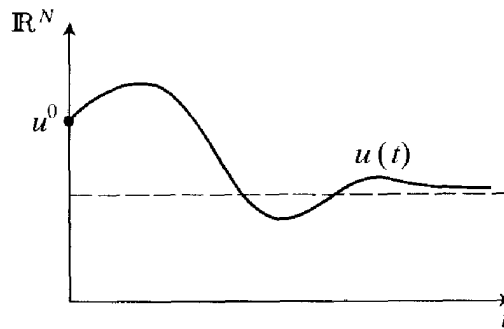$$u(t) = (u_1(t), \ldots, u_N(t)) \in \mathbb{R}^N, \quad t \in \mathbb{R}.$$

Fig. 5.1. Time diagram

We will also assume that the function $u(t)$ is determined by a dynamical system, i.e., a first order autonomous ordinary differential equation

$$\dot{u}(t) = f(u(t)). \tag{1.1}$$

Here the function $f : \mathbb{R}^N \to \mathbb{R}^N$ describes the mechanism of the underlying system and we assume it to be sufficiently smooth. The unique solution of the initial value problem

$$\dot{u} = f(u), \quad u(0) = u^0 \in \mathbb{R}^N \tag{1.2}$$

exists in some maximal open interval $J(u^0) \subset \mathbb{R}$. It will be denoted by $u(t)$ or $\Phi(t, u^0)$ or $\Phi(t, u^0, f)$, if the dependence on u^0 or f is of importance. For fixed t, the map

$$u^0 \to \Phi(t, u^0)$$

is called the *t-flow* of the system (1.1). This notion is made clear in fluid dynamics (cf. Kreiss and Lorenz[62], Chapter 1.2). There $f(u)$ denotes the velocity field at position u, so that a particle starting at position u^0 at time $t = 0$ will be at position $\Phi(t, u^0)$ at time t. Correspondingly, the curve

$$\gamma(u^0) = \{\Phi(t, u^0) : t \in J(u^0)\} \tag{1.3}$$

is called the *orbit* or the *trajectory of* u^0.

There are essentially two ways of visualizing the solutions of (1.2), either in a *time diagram*, where $u(t)$ or some functional of it is plotted versus time, or in a *phase diagram*, where the orbits are drawn (see Figures 5.1 and 5.2). The basic problem in dynamical systems is to describe the asymptotic behaviour

$$\Phi(t, u^0) \to ? \text{ as } t \to \infty$$

Fig. 5.2. Phase diagram
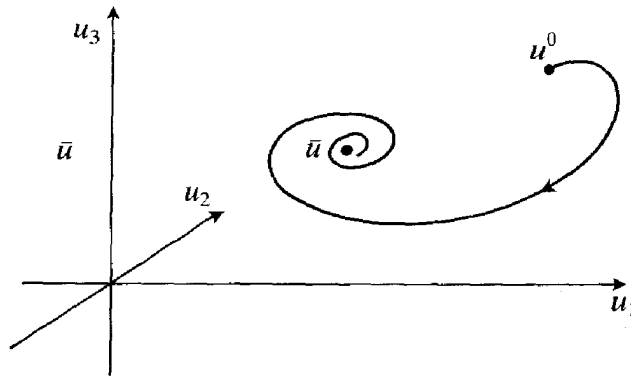
for as many initial values u^0 as possible. In some sense this asymptotic behaviour is captured by the *ω-limit set*

$$\omega(u^0) = \{v \in \mathbb{R}^N : \Phi(t_k, u^0) \to v \text{ as } k \to \infty \text{ for some sequence } t_k \to \infty\}.$$

The simplest case occurs if the solution becomes stationary, i.e.

$$\Phi(t, u^0) \to \bar{u} \text{ as } t \to \infty.$$

Then obviously $\omega(u^0) = \{\bar{u}\}$ and $f(\bar{u}) = 0$. This case is shown in Figures 5.1 and 5.2. Any vector $\bar{u} \in \mathbb{R}^N$ which satisfies $f(\bar{u}) = 0$ is called a *stationary point* or a *steady state*.

5.1.2 Two numerical approaches

The numerical analysis of the longtime behaviour of the flow Φ usually follows two complementary approaches:

Methods of type I (sometimes called *direct methods*)

Set up and solve numerically so-called *defining equations* for possible ω-limit sets of (1.1).
For example, set up the stationary system $f(v) = 0$ and use Newton's method

$$v^{n+1} = v^n - [f'(v^n)]^{-1}f(v^n). \tag{1.4}$$

It is well-known, that this method converges locally; i.e., the sequence will converge to some stationary point $\bar{u}$, if v^0 is sufficiently close to $\bar{u}$ and if

$$f'(\bar{u}) \text{ is nonsingular .} \tag{1.5}$$

Once a stationary point has been found, we may also determine its stability characteristics. If, in addition, the system has parameters we may continue this point into a branch of stationary points and detect singular points at which the stability characteristics change (see section 5.1.5 below).

Methods of type II (sometimes called *indirect methods*)

Solve the initial value problem (1.2) by some numerical integration method. In the simplest case this may be a one-step method with constant step size h

$$u^{n+1} = \varphi(h, u^n), \quad n = 0, 1, 2, \ldots, \quad u^0 \in \mathbb{R}^N. \tag{1.6}$$

For example $\varphi(h, u) = u + hf(u)$ in the case of Euler's method. The mapping $\varphi(h, \cdot)$ is the *discrete h-flow*, which is taken as an approximation of the continuous h-flow $\Phi(h, \cdot)$. A method of order p is obtained, if

$$\varphi(h, v) = \Phi(h, v) + O(h^{p+1}) \tag{1.7}$$

holds uniformly in some bounded set $\Omega \subset \mathbb{R}^N$ which contains the forward orbit $\{\Phi(t, u^0) : t \geq 0\}$. If, in addition, $\varphi(h, \cdot)$ has a uniform Lipschitz constant L in Ω, then classical estimates of the global discretization error are of the form (see e.g. Isaacson and Keller[52])

$$\|u(nh) - u^n\| \leq C \, h^p e^{Lnh}. \tag{1.8}$$

Clearly, these estimates becomes useless if $L > 0$ and $nh \gg 1$. One might then ask, if there are systems for which (1.8) can be shown to hold with $L = 0$ or even $L < 0$. This is in fact the case (see e.g. Stetter[93, Chapter 3.5]), however, the assumptions on the system usually require that all trajectories converge to one and the same stable stationary point. If we are also interested in unstable phenomena, then there will be some exponential divergence of trajectories (at least locally) and (1.8) cannot hold with $L \leq 0$. Therefore, we think, one should rather ask completely different questions, such as the following:

- Define the *discrete ω-limit set* of the numerical sequence u^n from (1.6) as

$$\omega_h(u^0) = \{v \in \mathbb{R}^N : u^{n_k} \to v \text{ as } k \to \infty \text{ for some sequence } n_k \to \infty\}.$$

Can anything be said about the distance between $\omega(u^0)$ and $\omega_h(u^0)$?

- Can we obtain the estimate (1.8) with $L \leq 0$ if we allow different initial values for the discrete and the continuous trajectories?
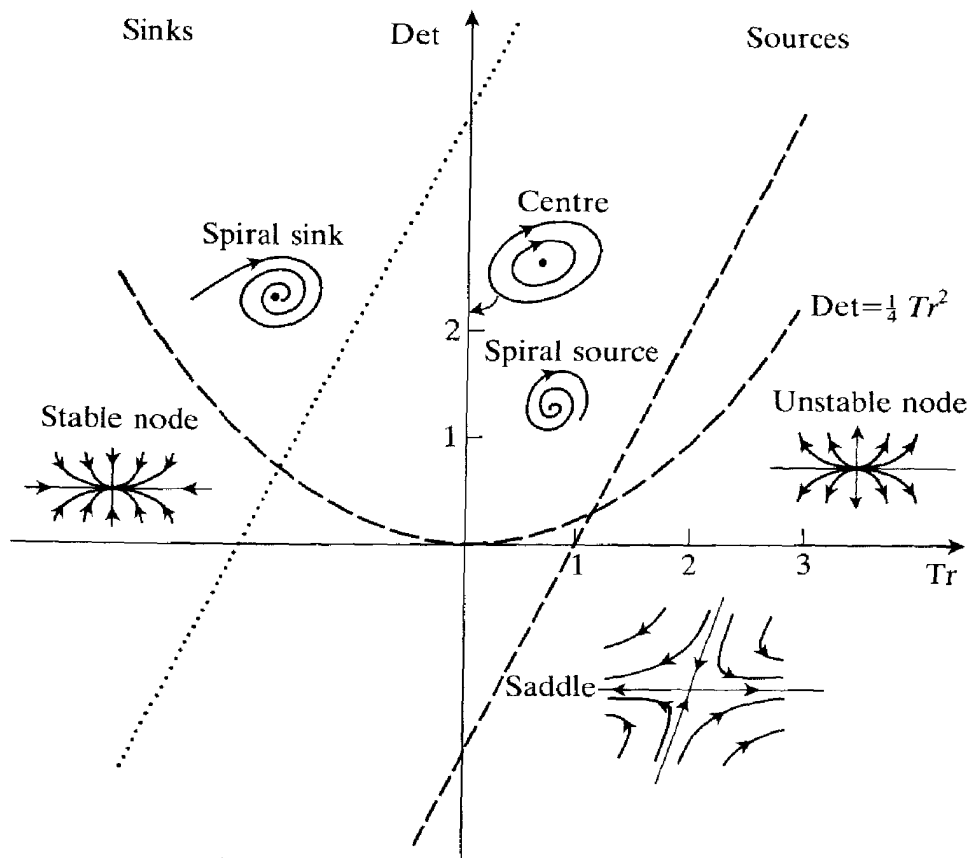
Fig. 5.3. Phase diagrams of 2-dimensional linear systems

This topic will be taken up in the last chapter. There we will concentrate on some positive answers for sufficiently small h. We notice, however, that there is also a growing literature which discusses the failures in the asymptotic behaviour of the numerical sequence u^n if h increases (see e.g., Brezzi, Fujii and Ushiki[17], Sanz-Serna[85], Stuart [96], Iserles, Peplow and Stuart[53]). Indirect methods usually provide some information on the *global* behaviour of trajectories for a few initial values. In contrast to this, direct methods only give some *local* information, which, however, is valid for a solid neighbourhood of initial values. In the following we will be concerned with these direct methods.

5.1.3 Some examples

The following three examples have been selected in order to demonstrate certain dynamic features and the typical structure of large dynamical systems ($N \gg 1$). A great variety of further examples can be found in the books cited at the beginning of this chapter.

Example 1

$$\dot{x} = y, \quad \dot{y} = 1 + y - x^2 + xy. \tag{1.9}$$

This is a seemingly simple example in 2 dimensions with $u = (x, y)$. There are two stationary points $(-1, 0)$ and $(1, 0)$.

Example 2 The linear two-dimensional system

$$\dot{u} = Au, \quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \tag{1.10}$$

The phase portrait depends on the eigenvalues of A

$$\mu_{\pm} = \frac{1}{2}(Tr \pm \sqrt{Tr^2 - 4\, Det}), \quad Tr = a + d, \quad Det = ad - bc$$

and the various cases are best shown in a Tr-Det diagram as in Figure 5.3 (see Hirsch see Smale[48], Chapter 5). The two lines shown will be used in later examples.

Example 3   Diffusion-reaction systems

$$\begin{aligned} v_t &= Dv_{xx} + g(x, v), & 0 \leq x \leq 1, & \quad t \geq 0 \\ v(x, 0) &= v^0(x), & 0 \leq x \leq 1 \\ v(0, t) &= \gamma_0, & v(1, t) = \gamma_1, & \quad t \geq 0. \end{aligned}$$

Here $v(x, t) \in \mathbb{R}^n$ is a vector describing the concentrations of n reactants at time t and location $x \in [0, 1]$. The reaction term g couples the various concentrations (in the case of bimolecular reactions it is a quadratic term in v), while D is a diagonal matrix containing the diffusion coefficients. The standard method of lines approach introduces a spatial grid $x_i = i\Delta x$, $\Delta x = 1/(m + 1)$ and approximates the parabolic system above by

$$v_t(x_i, t) = (\Delta x)^{-2} D(v(x_{i-1}, t) - \tag{1.11}$$
$$2v(x_i, t) + v(x_{i+1}, t)) + g(x_i, v(x_i, t)), \quad i = 1, \ldots m.$$

Here $v(x_0, t)$ and $v(x_{m+1}, t)$ are replaced by the given boundary values. Introducing the vector

$$u(t) = (v(x_1, t), \ldots, v(x_m, t)) \in \mathbb{R}^{mn}$$

yields a dynamical system of the form (1.1) where the Jacobian $f'(u)$ is a large matrix with tridiagonal block structure
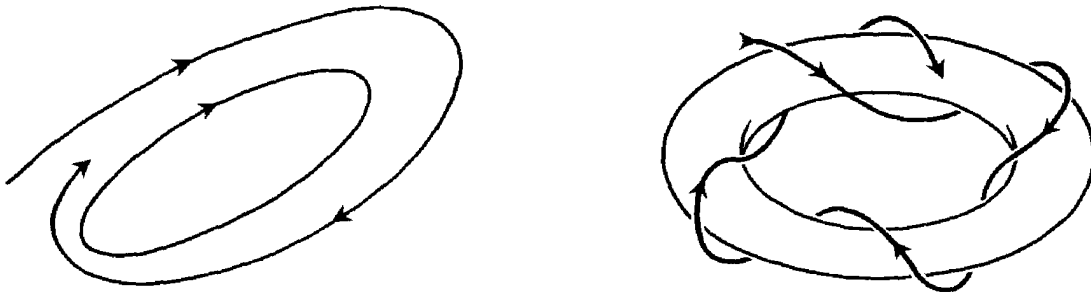
Fig. 5.4. A periodic orbit and an invariant torus

$$f'(u) = \begin{bmatrix} \ddots \\ & \ddots \\ & & \ddots \end{bmatrix} .$$

This example opens up the road to partial differential equations and it suggests that direct numerical methods should take advantage of the sparsity of $f'(u)$.

5.1.4 Fundamental notations and results

At the beginning of this chapter we referred to a few books on numerical methods for dynamical systems. Similarly, we mention here some monographs on the theory of dynamical systems Hale[44], Arnold[5], Hirsch and Smale[48], Irwin[51], Chow and Hale[20], Guckenheimer and Holmes[43], Amann[3]. These will be freely used without giving the particular reference at any instant.

Given a dynamical system (1.1), an arbitrary set $M \subset \mathbb{R}^N$ is called *invariant* if

$$\Phi(t, u^0) \in M \quad \text{for all} \quad t \in \mathbb{R} \quad \text{whenever} \quad u^0 \in M.$$

If this holds only for $t \geq 0$, then M is called *positively invariant*. It is easily seen that any ω-limit set $\omega(u^0)$ is invariant and closed. Hence it is also compact, if the positive trajectory stays bounded.
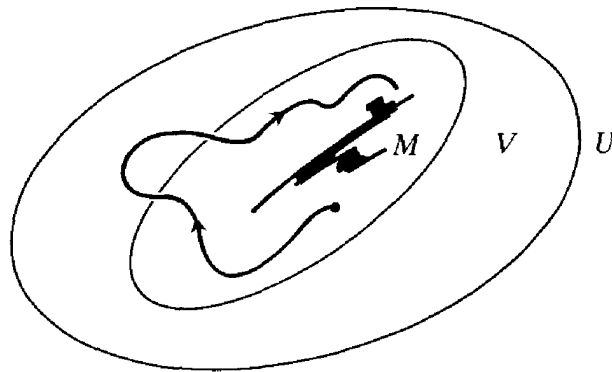
Fig. 5.5. Stability of a compact invariant set

The most frequent compact invariant sets next to stationary points are *periodic orbits* and *invariant tori* (see Figure 5.4). Suppose that $\Phi(T, u^0) = u^0$ for some $T > 0$ and that T is the smallest number with this property. Then

$$\gamma(u^0) = \{\Phi(t, u^0) : 0 \leq t \leq T\}$$

is a periodic orbit of period T and we have

$$\Phi(t + T, v) = \Phi(t, v) \quad \text{for all} \quad t \in \mathbb{R}, \quad v \in \gamma(u^0).$$

An invariant torus is of the form

$$M = \{P(\Theta_1, \Theta_2) : 0 \leq \Theta_1 \leq 2\pi, 0 \leq \Theta_2 \leq 2\pi\}$$

where $P : \mathbb{R}^2 \to \mathbb{R}^N$ is 2π-periodic in Θ_1 and Θ_2 and where

$$\Phi(t, P(\Theta)) = P(\Phi_M(t, \Theta)), \quad t \in \mathbb{R}, \Theta = (\Theta_1, \Theta_2)$$

for some mapping Φ_M. Notice that the invariant set M can no longer be parametrized by time. Some nontrivial dynamics on M remains, given by the reduced flow $\Phi_M(t, \cdot)$.

Let $M \subset \mathbb{R}^N$ be some compact invariant set. This set can only be "observed" in a real system, i.e., in mathematical terms it appears as an ω-limit set for sufficiently many initial values, if it attracts nearby trajectories or at least if it keeps them close. This motivates the following definition.

The set M is called *stable* (compare Figure 5.5), if for any neighbourhood U of M there exists another neighbourhood V of M such that

$$u^0 \in V \Rightarrow \Phi(t, u^0) \in U \quad \text{for all} \quad t \geq 0.$$
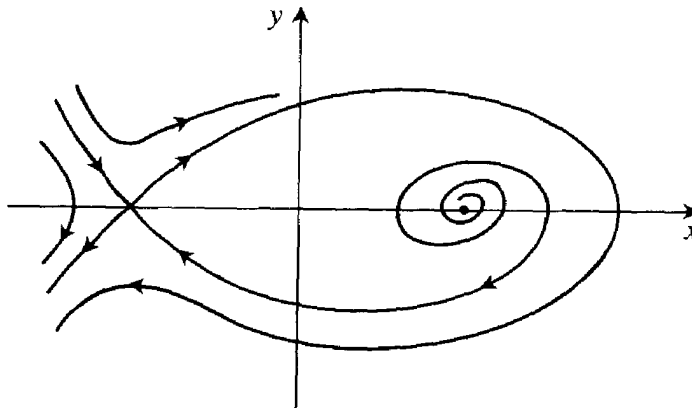
Fig. 5.6. Global phase diagram for example 1

M is called *unstable*, if it is not stable. Finally, M is called *asymptotically stable* if it is stable and if there exists a neighbourhood U of M such that

$$u^0 \in U \Rightarrow \text{dist}(\Phi(t,u^0),M) \to 0 \quad \text{as} \quad t \to \infty.$$

The basic stability result for stationary points is

Theorem 1.1. *Let $\bar{u} \in \mathbb{R}^N$ be a stationary point of $\dot{u} = f(u)$. Then $\bar{u}$ is asymptotically stable if $Re\ \mu < 0$ for all eigenvalues $\mu \in C$ of $f'(\bar{u})$, and it is unstable, if $Re\ \mu > 0$ for at least one eigenvalue of $f'(\bar{u})$.*

As a consequence, we find for our example 2(see Figure 5.3) that the origin is asymptotically stable, if (Tr, Det) is in the open upper left quadrant, and it is unstable if Tr > 0 or Det < 0. The center occuring on the semi-axis Tr = 0, Det > 0 is stable but not asymptotically stable.

The stationary point $\bar{u} \in \mathbb{R}^N$ of (1.1) is called *hyperbolic*, if $f'(\bar{u})$ has no eigenvalue on the imaginary axis. In this case the phase diagram of the nonlinear system resembles at least locally that of the linearized system according to the following theorem.

Theorem 1.2. *(Hartman, Grobman). Let $\bar{u} \in R^N$ be a hyperbolic stationary point. The flows of $\dot{u} = f(u)$ and $\dot{u} = f'(\bar{u})u$ are locally flow equivalent, more precisely there exists a homeomorphism h from some neighbourhood of 0 onto some neighbourhood of $\bar{u}$ such that*

$$\Phi(t,h(u^0),f) = h(\Phi(t,u^0,f'(\bar{u}))) = h(e^{tf'(\bar{u})}u^0).$$
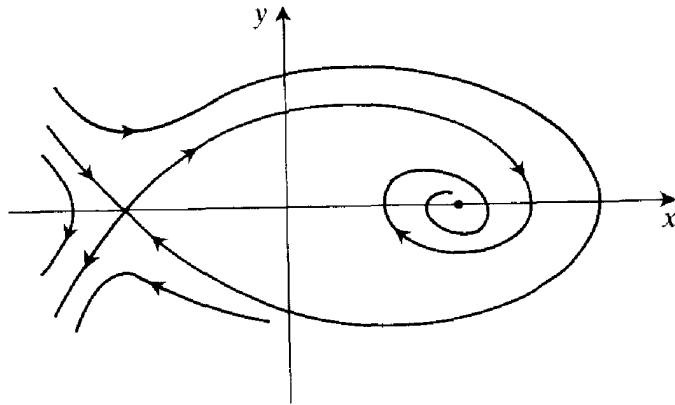
Fig. 5.7. Global phase diagram for example 1(-)

Let us apply these results to example 1 in 5.1.3. We have

$$f'(x,y) = \begin{pmatrix} 0 & 1 \\ -2x+y & 1+x \end{pmatrix}, \ \text{Tr} = 1+x, \ \text{Det} = 2x - y.$$

Hence, Tr $= 0$, Det $= -2$ at $(x,y) = (-1,0)$ and Tr $= 2$, Det $= 2$ at $(x,y) = (1,0)$.

Therefore, $(-1,0)$ is a saddle and $(1,0)$ is a spiral source. The global phase diagram is shown in Figure 5.6. We have included in Figure 5.7 the slightly modified example

Example 1(-)

$$\dot{x} = y, \ \dot{y} = 1 - 2y - x^2 + xy. \tag{1.12}$$

Here, $(-1,0)$ remains a saddle, but $(1,0)$ has turned into a spiral sink.

5.1.5 Parameters and bifurcations

In this section we consider dynamical systems with one parameter λ,

$$\dot{u} = f(u,\lambda). \tag{1.13}$$

Changing the parameter may drive the system from one asymptotic behaviour to another. At certain values of λ one type of invariant set (e.g., a stationary point) may loose its asymptotical stability and a new type of invariant set (e.g., a periodic orbit) may be created which takes over the

stability. In a loose sense these are the so-called *bifurcations*. There need not be an exchange of stability at a bifurcation. However, in applications this is the most important effect.

We briefly review here the various bifurcation phenomena in one parameter systems which connect stationary points, periodic orbits and tori. In Table 5.1 some typical stability assignments are shown using the following conventions (cf. Doedel and Kernevez[28]).

————————	stable stationary points
— — — — — — — — — —	unstable stationary points
• • • • • • • • • •	stable periodic orbits
○ ○ ○ ○ ○ ○ ○ ○ ○ ○	unstable periodic orbits
⊙ ⊙ ⊙ ⊙	stable tori

For a numerical analysis of these bifurcations we are confronted with the following tasks:

- detect a bifurcation point while following a branch of invariant objects
- accurately locate the bifurcation point by a *defining equation*
- create a good initial approximation for starting a branch of the new invariant objects (*branch switching*).

It has been pointed out by Seydel[87], Chapter 5.3, that in many practical problems the accurate location of bifuration points is not really necessary (some interpolation on the branch will be sufficient). However, it becomes important if we introduce a second parameter and try to follow a branch of bifurcation points. On such a branch we may well encounter a new bifurcation – a so-called *codimension 2 singularity* – and all the above questions arise again. We will treat in this paper only one such codimension 2 singularity – the so-called *Takens-Bogdanov singularity* or *B*-point (see e.g. Fiedler[34]). Even higher singularities have been detected for example by Khibnik, Bykov and Yablonskii[58], De Dier, Roose and Van Rompay[23] and Khibnik[59].

Let us finally add an example of a torus bifurcation.

Example 4

$$\dot{r} = r(\lambda - r^2), \quad \dot{\Theta}_1 = a > 0, \quad \dot{\Theta}_2 = b. \tag{1.14}$$

Here Θ_1, Θ_2 are assumed to be 2π-periodic, i.e., $\Theta_1, \Theta_2 \in S_{2\pi} := \mathbb{R}/2\pi\mathbb{Z}$. For the r-equation an asymptotically stable stationary point $\sqrt{\lambda}$ bifurcates from the origin at $\lambda = 0$. If we transform (1.14) into Cartesian coordinates via

$$(x, y, z) = ((1 - r\cos\Theta_2)\cos\Theta_1, \ (1 + r\cos\Theta_2)\sin\Theta_1, \ r\sin\Theta_2)$$

bifurcation diagram	**bifurcation name**
	saddle node or *turning point* a parabola-like branch of stationary solutions
	Hopf bifurcation a branch of periodic orbits created out of stationary solutions
	turning point of period orbits a parabola-like branch of periodic orbits
	homoclinic bifurcation a branch of periodic orbits attaining infinite period
	period doubling bifurcation a branch of periodic orbits with approximately doubled period created out of a periodic orbit
	torus bifurcation a branch of invariant tori created out of a periodic orbit

Table 5.1. Various bifurcation phenomena

we find that the periodic orbit

$$\{(\cos(at), \sin(at), 0) : 0 \le t \le 2\pi/a\}$$

bifurcates at $\lambda = 0$ into an asymptotically stable torus

$$\left\{(1 - \sqrt{\lambda} \cos \Theta_2) \cos \Theta_1, \right.$$

$$\left. (1 + \sqrt{\lambda} \cos \Theta_2) \sin \Theta_1, \sqrt{\lambda} \sin \Theta_2) : 0 \le \Theta_1, \Theta_2 \le 2\pi\right\}.$$

5.2 The direct computation of stationary points, periodic orbits and more general invariant manifolds

5.2.1 Stationary points

The basic features of Newton's method for solving the stationary equation $f(u) = 0$ have already been mentioned in 1.2. We notice here that the nonsingularity assumption on $f'(\bar{u})$ (see (1.5)) is slightly weaker then the hyperbolicity assumption which guarantees the persistence of the local phase diagram (Theorem 1.2). Further details on Newton's method, update methods and methods for following branches can be found in Ortega and Rheinboldt[74], Stoer and Bulirsch[95], Rheinboldt[80] Seydel[87] and Allgower and Georg[1] The stability of $\bar{u}$ can be analysed by calculating the eigenvalues of $f'(\bar{u})$ (see Theorem 1.1).

5.2.2 Periodic orbits

In order to compute a periodic orbit we have to find a period $T > 0$ and a solution $u(t) \in \mathbb{R}^N$ of the boundary value problem

$$\dot{u} = f(u), \quad t \in [0, T], \quad u(0) = u(T). \tag{2.1}$$

Since T is one of the unknowns we introduce the scaled function $v(t) = u(tT)$, $t \in [0, 1]$, for which we have the boundary value problem

$$\dot{v} = T f(v), \quad t \in [0, 1] \tag{2.2}$$

$$v(0) - v(1) = 0. \tag{2.3}$$

Here we have $N + 1$ unknowns $v(t), T$, but only N boundary conditions. In fact, if $v(t)$ is a solution of (2.2, 2.3), then we can extend it 1-periodically to $t \in \mathbb{R}$ and find that any phase shifted function $v(t + q)$, $q \in \mathbb{R}$ also solves
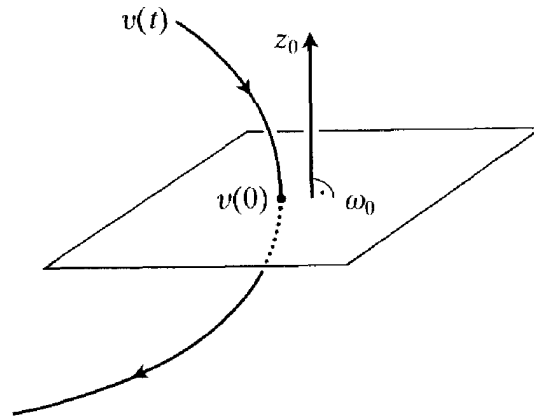
Fig. 5.8. Classical phase condition

(2.2, 2.3). This arbitrariness can be eliminated by imposing an $(N + 1)$-st boundary condition, the so-called *phase condition*. We take it in the general form

$$\Psi(v) = 0, \tag{2.4}$$

where $\Psi : C_1^1[0,1] \to \mathbb{R}$ is any functional and $C_1^1[0,1]$ denotes the space of 1-periodic C^1 functions from $[0,1]$ to $\mathbb{R}^N$. The *classical phase condition* is obtained if we fix $v(0)$ in a hyperplane through some approximate vector w_0 and orthogonal to some direction z_0 (see Figure 5.8), i.e.,

$$\Psi(v) = z_0^T (v(0) - w_0). \tag{2.5}$$

A good choice usually is $z_0 = f(w_0)$. Finally, adding the equation $\dot{T} = 0$, we may now apply any of the available boundary value solvers to (2.2, 2.3, 2.4) (see e.g., Ascher, Mattheij and Russell[6], Seydel[87]). These codes usually do not allow to take advantage of some sparsity of f' (cf. 5.1.3, Example 3), so that specialized programs have been developed (Holodniok, Knedlik and Kubiček[49]).

An integral phase condition has been set up and implemented by Doedel[27] (see also Doedel and Kernevez[28]). In continuation problems this condition usually allows for larger step sizes and is more robust than (2.5). It has the form

$$\Psi(v) = \int_0^1 z_0^T(t)(v(t) - v_0(t))\, dt, \tag{2.6}$$

where v_0 is an approximation from the predictor and $z_0 = \dot{v}_0 \approx f(v_0)$. The motivation for (2.6) comes from the following:

Lemma 2.1. *Suppose that $v_0 \in C_1^1[0,1]$ is nonconstant. Then there is a neighbourhood U of v_0 in $C_1^1[0,1]$, such that for any $v \in U$ the L_2-distance*

$$\int_0^1 \|v(t+q) - v_0(t)\|_2^2 \, dt, \quad \|\cdot\|_2 = \text{Euclidean norm} \qquad (2.7)$$

has a unique local minimum at some $q = q(v)$ close to zero. At the minimum we have

$$\int_0^1 \dot{v}_0^T(t)(v(t+q) - v_0(t)) \, dt = 0.$$

Proof. Let $F(q,v)$ denote the L_2-norm from (2.7). Then we find

$$\frac{\partial F}{\partial q}(q,v) = 2 \int_0^1 \dot{v}(t+q)^T(v(t+q) - v_0(t)) \, dt.$$

Using the periodicity of v and partial integration we obtain

$$\frac{\partial F}{\partial q}(q,v) = 2 \int_0^1 \dot{v}_0^T(t) v(t+q) \, dt.$$

Therefore, $\frac{\partial F}{\partial q}(0, v_0) = 0$ and

$$\frac{\partial^2 F}{\partial q^2}(0, v_0) = 2 \int_0^1 \|\dot{v}_0(t)\|_2^2 \, dt > 0.$$

We may now apply the implicit function theorem to the equation $\frac{\partial F}{\partial q}(q,v) = 0$ and find all our assertions. ∎

Determining the stability of a periodic orbit can be a considerable numerical task. One has to calculate the so-called *monodromy matrix* $Y(T) \in \mathbb{R}^{N,N}$ which is the T-value of the fundamental matrix $Y(t)$, $0 \le t \le T$ of the system

$$\dot{Y}(t) = f'(u(t))Y(t), \quad 0 \le t \le T, \quad Y(0) = I. \qquad (2.8)$$

The eigenvalues of $Y(T)$ are called *Floquet multipliers*. By differentiating (2.1) we easily find

$$Y(t)\dot{u}(0) = \dot{u}(t) \quad \text{and} \quad Y(T)\dot{u}(0) = \dot{u}(T) = \dot{u}(0).$$

Hence 1 is always a Floquet multiplier and stability is determined by the remaining ones (cf. Hirsch and Smale[48], Amann[3]).

Theorem 2.2. *Let* $\gamma = \{u(t) : 0 \leq t \leq T\}$ *be a T-periodic orbit of* $\dot{u} = f(u)$ *with monodromy matrix* $Y(T)$*. Then the orbit is asymptotically stable if 1 is a simple eigenvalue of* $Y(T)$ *and if* $|\mu| < 1$ *for all other eigenvalues* μ*. The orbit is unstable if* $|\mu| > 1$ *for at least one Floquet multiplier* μ*.*

The monodromy matrix can often be determined as a by-product of the numerical solution of the boundary value problem (2.2, 2.3, 2.4) (see Doedel and Kernevez[28], Seydel[87], Chapter 7). This is possible because the discretization of (2.2, 2.3, 2.4) is linearized during some Newton step and the matrix obtained is close to a discretization of the linearized system (2.8). Doing some kind of 'forward integration' with this system provides an approximation for $Y(T)$. However, it is also well-known that this shooting type approach completely fails if there are Floquet multipliers which are very small or very large in modulus (cf. Doedel and Kernevez[28], Stiefenhofer[94]). This *stiff periodic case* typically occurs with relaxation oscillations.

We finally mention a result of Keller and Jepson[57]. It characterizes the admissible phase conditions (2.4) which lead to a regular boundary value problem (2.2, 2.3, 2.4). By *regular* we mean here that if we write (2.2, 2.3, 2.4) as an operator equation

$$F(v, T) = (\dot{v} - T \ f(v), v(0) - v(1), \Psi(v)) = 0$$

where $F : C^1[0, 1] \times \mathbb{R} \to C^0[0, 1] \times \mathbb{R}^{N+1}$, then we require that the Frechét derivative of F (in some suitable norms) at the solution is a homeomorphism.

Theorem 2.3. *Let* $u(t)$ *be a solution of (2.1) and let* $v(t) = u(tT)$*. Then (2.2, 2.3, 2.4) is a regular boundary value problem for* (v, T) *if and only if the following two conditions hold*

(i) 1 is a simple Floquet multiplier

(ii) $\Psi'(v)\dot{v} \neq 0$.

Condition (ii) is a rather mild requirement; for the classical phase condition (2.5) it means $z_0^T \dot{v}(0) \neq 0$, while (2.6) requires

$$\int_0^1 z_0^T(t)\dot{v}(t) \, dt \neq 0.$$

Further, as in the stationary case condition (i) is weaker than the *hyperbolicity* of the orbit, which requires that 1 is not only a simple Floquet multiplier, but also the only one on the unit circle. Again hyperbolicity guarantees the persistence of the dynamic behaviour under perturbations.

5.2.3 More general invariant manifolds

Smooth invariant manifolds are an important tool in the analysis of dynamical systems. On the one hand, these are applied for lowering the dimensionality of the system without loosing the ω-limit sets (or attractors) under investigation. Examples are:

- *center manifolds* (see e.g. Carr[18], Guckenheimer and Holmes[43])
- *inertial manifolds* (e.g. Temam[98]).

On the other hand, invariant manifolds also serve to understand the dynamics in low-dimensional systems by either bounding domains of attraction or appearing as limit sets themselves such as

- *separatrices* consisting of *stable and unstable manifolds*
- *invariant tori.*

The numerical approximation of these invariant manifolds has been undertaken just recently (see Kevrekidis, Aris, Schmidt and Pelikan[60], van Veldhuizen[99], Foias, Jolly, Kevrekidis, Sell and Titi[35], Doedel and Friedman[29,30,31], Dieci, Lorenz and Russell[25], Beyn[11]). Some special separatrices – the homoclinic orbits – will be discussed in the next chapter. In this section we outline the method of Dieci, Lorenz and Russell[25] (see also Lorenz and Van de Velde[70]) for calculating invariant manifolds in the special case of a two-dimensional torus.

They assume, that the given dynamical system has been subject to a coordinate transformation $u \rightarrow (\Theta, R)$, after which it takes the form

$$\dot{\Theta} = f(\Theta, R), \quad \dot{R} = g(\Theta, R). \tag{2.9}$$

Here $R \in \mathbb{R}^{N-2}$ and $\Theta \in T^2 := (\mathbb{R}/2\pi\mathbb{Z})^2$ is already a toroidal coordinate. Our example 4 (section 5.1.5) is of this type with f being constant and g depending only on R. We look for an invariant manifold of the form

$$M = \{(\Theta, r(\Theta)) : \Theta \in T^2\}. \tag{2.10}$$

Decomposing the flow $\Phi = (\Phi_\Theta, \Phi_R)$ according to (2.9) we may write the invariance condition as

$$\Phi_R(t, \Theta, R) = r(\Phi_\Theta(t, \Theta, R)) \quad \text{for } (\Theta, R) \in M.$$

Differentiating this identity with respect to t and setting $t = 0$ yields

$$g(\Theta, R) = r'(\Theta)f(\Theta, R) = f_1(\Theta, R)\frac{\partial r}{\partial \Theta_1}(\Theta) + f_2(\Theta, R)\frac{\partial r}{\partial \Theta_2}(\Theta).$$

Inserting $R = r(\Theta)$ gives the following first order system of nonlinear partial differential equations for the function $r : T^2 \to \mathbb{R}^{N-2}$

$$g(\Theta, r) = f_1(\Theta, r)\frac{\partial r}{\partial \Theta_1} + f_2(\Theta, r)\frac{\partial r}{\partial \Theta_2}. \qquad (2.11)$$

The requirement that r is a smooth function of $\Theta \in T^2$ can be written as

$$\Theta \in [0, 2\pi] \times [0, 2\pi], r(0, \Theta_2) = r(2\pi, \Theta_2), \ r(\Theta_1, 0) = r(\Theta_1, 2\pi). \qquad (2.12)$$

The boundary value problem (2.11), (2.12) is discretized with *central differences* (*leap frog*)

$$g(\Theta, r(\Theta)) = f_1(\Theta_1 r(\Theta))D_1 r(\Theta) + f_2(\Theta, r(\Theta))D_2 r(\Theta), \ \Theta \in \Omega_h \qquad (2.13)$$

where

$$\Omega_h = \{(n_1 h_1, n_2 h_2) : n_j \in Z(\bmod N_j), \ j = 1, 2\}, \ h_j = \frac{2\pi}{N_j}$$

and

$$D_1 r(\Theta) \ = \ \frac{1}{2h_1} \left(r(\Theta_1 + h_1, \Theta_2) - r(\Theta_1 - h_1, \Theta_2) \right)$$

$$D_2 r(\Theta) \ = \ \frac{1}{2h_2} \left(r(\Theta_1, \Theta_2 + h_2) - r(\Theta_1, \Theta_2 - h_2) \right).$$

The periodicity condition is built into the definition of Ω_h. Now Newton's method can be applied to (2.13), and the linear systems arising in each step are of block tridiagonal form (cf. 5.1.3) with an additional block in the upper right and lower left corner.

If these linear systems are solved in a shooting type manner (called *compactification*), then ill-conditioned matrices arise, and a modification of the discretization avoiding these failures is proposed in Dieci, Lorenz Russell[25]. The compactification of these linear systems also elucidates the relations to another approach for invariant tori (see van Veldhuizen[99]). In that method the torus is computed via its intersection with a given plane, which is an invariant curve for the Poincaré map. This increases the geometric flexibility of the method if compared to the rather restrictive pre-transformation (2.9). On the other hand, the invariant circle methods rely to some extent on the asymptotic stability of the torus and the dynamics on it, while the PDE approach (2.11), (2.13) seems to be independent of it.

Of course, all these methods run into difficulties if the torus looses smoothness and breaks up. This is probably one of the possible routes to chaos (cf. Newhouse, Ruelle and Takens[73]).
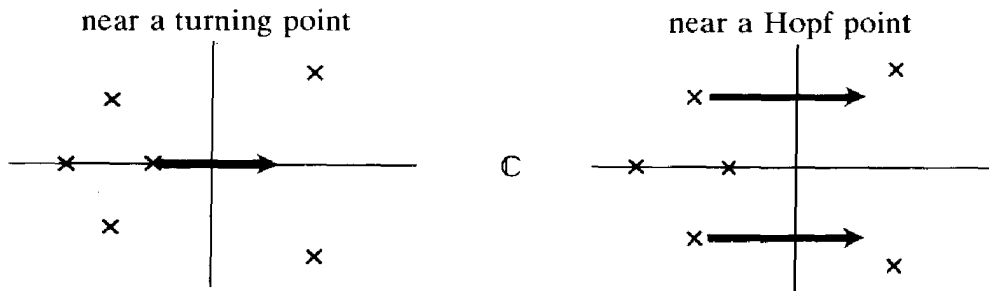
near a turning point   near a Hopf point

Fig. 5.9. Eigenvalues of f_u

5.3 Singular points in one-parameter systems

5.3.1 The loss of hyperbolicity on a branch

In this chapter we take up the questions of detecting and locating singular points in one-parameter systems (cf. section 5.1.5)

$$\dot{u} = f(u, \lambda), \quad \lambda \in \mathbb{R}, \quad u(t) \in \mathbb{R}^N. \tag{3.1}$$

Any stationary point of (3.1), which is not hyperbolic, will be called *singular*. Let $(u(s), \lambda(s))$ be a smooth branch of stationary points parametrized by $s \in (-s_0, s_0) \subset \mathbb{R}$, $s_0 > 0$. Looking at the spectrum of $f_u(u(s), \lambda(s))$, we can imagine basically two ways in which the stationary points loose hyperbolicity. Either a real eigenvalue crosses zero or a pair of complex conjugate eigenvalues crosses the imaginary axis (see Figure 5.9). In the first case we have a *turning point* (or a *saddle node* in the language of dynamical systems), and in the second case we have a *Hopf point*.

5.3.2 Turning points (saddle nodes)

The situation near a turning point is described in the following Theorem:

Theorem 3.1. *Let* $(u(s), \lambda(s))$, $s \in (-s_0, s_0)$ *be a smooth stationary branch of (3.1) with* $(u'(s), \lambda'(s)) \neq 0$ *for all* s. *Further assume that* $f_u^0 := f_u(u(0), \lambda(0))$ *has a simple eigenvalue 0 with eigenvector* ϕ_0 *normalized by* $\phi_0^T \phi_0 = 1$ *and that* $(f_u^0 \ f_\lambda^0)$ *has rank* N. *Then* $\lambda'(0) = 0$ *holds and the following conditions are equivalent*

(i) $\lambda''(0) \neq 0$

(ii) $\mu'(0) \neq 0$, *where* $\mu(s)$ *denotes the smooth continuation of the eigenvalue 0 for* $f_u^s := f_u(u(s), \lambda(s))$

(iii) $(u(0), \lambda(0), \phi_0)$ *is a regular solution of the defining equation*

$$T(u, \lambda, \phi) = \begin{pmatrix} f(u, \lambda) \\ f_u(u, \lambda)\phi \\ \phi^T\phi - 1 \end{pmatrix} = 0, \qquad (3.2)$$

i.e., $T'(u(0), \lambda(0), \phi_0)$ *is nonsingular.*

Remark: If any of these three conditions is satisfied, then $(u(0), \lambda(0))$ is called a *quadratic* (or *simple*) *turning point*. The obvious reason is the geometric condition (i), according to which the branch is locally a parabola either turning to the right or to the left (see 5.1.5). Condition (i) is the characterization in terms of eigenvalues and condition (iii) is the first example of a defining equation given by Seydel[86] and further analyzed by Moore and Spence[72]. We will discuss a special aspect of defining systems in the next section, but for a broad overview we refer to Seydel[87]. For later reference we indicate here the proof of (i) $\Leftrightarrow$ (ii).

Proof. (i) $\Leftrightarrow$ (ii)   Differentiating

$$f(u(s), \lambda(s)) = 0$$

yields

$$f_u^s u'(s) + f_\lambda^s \lambda'(s) = 0.$$

Taking $s = 0$ we obtain from our assumptions that $\lambda'(0) = 0$ and $u'(0) = c\ \phi_0$ for some $c \in \mathbb{R}$. We differentiate again with respect to s and find at $s = 0$,

$$c^2 f_{uu}^0 \phi_0^2 + f_u^0 u''(0) + f_\lambda^0 \lambda''(0) = 0.$$

Consequently, condition (i) is equivalent to

$$f_{uu}^0 \phi_0^2 \notin R(f_u^0) \qquad (3.3)$$

where $R(f_u^0)$ denotes the range of f_u^0.
Similarly, the equivalence of condition (ii) and (3.3) can be shown by differentiating the following eigenvalue equation at $s = 0$

$$f_u(u(s), \lambda(s))\phi(s) = \mu(s)\phi(s),$$

where $\mu(0) = 0$, $\phi(0) = \phi_0$.   ∎

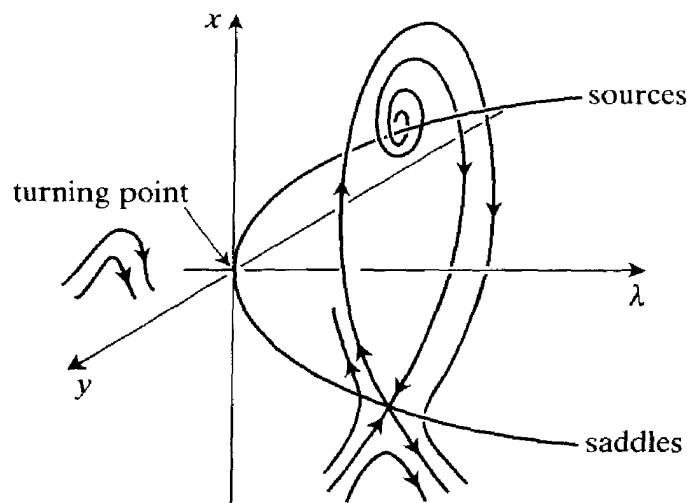Let us illustrate the phase diagrams near a turning point by introducing a parameter λ into example 1 (see (1.9))

Fig. 5.10. Phase diagrams for Example 1(λ)

Example 1(λ)

$$\dot{x} = y, \quad \dot{y} = \lambda + y - x^2 + xy. \tag{3.4}$$

Here the stationary branch is

$$(x(s), y(s), \lambda(s)) = (s, 0, s^2)$$

and for the linearization f_u^s we find

$$\mathrm{Tr}(s) = 1 + s, \quad \mathrm{Det}(s) = 2s.$$

This is shown as a dashed line in Figure 5.3. The change of phase diagram with λ is illustrated in Figure 5.10. Notice that, according to Figure 5.3, the spiral source at $(\sqrt{\lambda}, 0)$ becomes an unstable node before coalescing with the saddle at $\lambda = 0$.

5.3.3 Defining equations

One Newton step for the defining equation (3.2) involves the solution of a linear system of dimension $2N + 1$, but, as Moore and Spence[72] showed, this can be reduced to 4 linear systems of dimension $N + 1$ with the same matrix. This matrix is nonsingular at the turning point and has the form

$$A(u, \lambda) = \begin{pmatrix} f_u(u, \lambda) & b_0 \\ c_0^T & 0 \end{pmatrix}, \quad b_0, c_0 \in \mathbb{R}^N. \tag{3.5}$$

This result clearly suggests replacing (3.2) right away by a system of dimension $N + 1$:

$$T(u, \lambda) = \begin{pmatrix} f(u, \lambda) \\ g(u, \lambda) \end{pmatrix} = 0, \tag{3.6}$$

where $g(u, \lambda) \in \mathbb{R}$ is implicitly defined through

$$A(u, \lambda) \begin{pmatrix} v(u, \lambda) \\ g(u, \lambda) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad v(u, \lambda) \in \mathbb{R}^N. \tag{3.7}$$

In fact, this is the approach proposed by Griewank and Reddien[41,42] Similar systems are given Abbott[2], Pönisch and Schwetlick[78], and even further reduced equations are considered in Jepson and Spence[55], Beyn[7]. Though many of these methods lead to comparable numerical effort, we think that the approach of Griewank and Reddien has several appealing features, conceptually as well as computationally:

(a) The function g can be used for detection as well as accurate location of a singular point. This generalizes to other singularities (see below).

(b) The system is written in such a way that the linear algebra of a Newton step suggests itself. In particular it can be seen that several linear systems with the same matrix $A(u, \lambda)$ or its adjoint have to be solved (see Lemma 3.2).

(c) If one wants to retain the original equation $f = 0$, then (3.6) is the minimal extension possible.

Let us explain the argument b) in more detail. First, we have to evaluate the derivative

$$g_z(z) = (g_u(u, \lambda), g_\lambda(u, \lambda)), \quad z = (u, \lambda)$$

which appears in a Newton step for (3.6). Here the following Lemma is useful (cf. Griewank and Reddien[41,42]). For later purposes we will formulate it for the case of $p \geq 1$ parameters.

Lemma 3.2. *Let $\Omega \subset \mathbb{R}^{N+p}$ be open and $f : \Omega \to \mathbb{R}^N$ be smooth such that*

$$A(z) := \begin{pmatrix} f_u(z) & B_0 \\ C_0^T & 0 \end{pmatrix} \in \mathbb{R}^{N+p,N+p}, \quad B_0, C_0 \in \mathbb{R}^{N,p} \text{ fixed} \tag{3.8}$$

is nonsingular for all $z = (u, \lambda) \in \Omega$. Define the functions

$$U, V : \Omega \to \mathbb{R}^{N,p} \quad \text{and} \quad G, \widetilde{G} : \Omega \to \mathbb{R}^{p,p}$$

by

$$A(z) \begin{pmatrix} V(z) \\ G(z) \end{pmatrix} = \begin{pmatrix} 0 \\ I_p \end{pmatrix}, \tag{3.9}$$

$$(U^T(z) \ \widetilde{G}(z))A(z) = (0 \ I_p). \tag{3.10}$$

Then the following relations hold in Ω

$$G = \widetilde{G} = -U^T f_u V \tag{3.11}$$

$$G_z = -U^T f_{uz} V. \tag{3.12}$$

Proof. Let us write down (3.9), (3.10) explicitly

$$f_u V + B_0 G = 0, \qquad C_0^T V = I_p$$
$$U^T f_u + \widetilde{G} C_0^T = 0, \qquad U^T B_0 = I_p.$$

Multiplying the first equation by U^T from the left and the third by V from the right immediately yields (3.11). The same operation on the derived terms gives

$$U^T f_{uz} V + U^T f_u V_z + G_z = U_z^T f_u V + U^T f_{uz} V + G_z = 0.$$

We then arrive at (3.12) by combining these formulas with the formula obtained by direct differentiation of (3.11). ∎

We notice that G_z can be easily evaluated from f_z by numerical differentiation, e.g., if $p = 1$, we may use

$$g_z(z) \sim -\frac{1}{h} U^T(f_z(u + hV, \lambda) - f_z(u, \lambda)). \tag{3.13}$$

In the Newton step for (3.6) we have to solve a linear system with

$$T'(u, \lambda) = \begin{pmatrix} f_u & f_\lambda \\ g_u & g_\lambda \end{pmatrix} (u, \lambda).$$

We now insist that this is done with the help of the matrix (3.5). One reason for this is that the user may provide a black box routine for solving with the bordered matrix (3.5) (or (3.8) in the general case). The following Lemma shows how to reduce the solution of one bordered linear system to the solution of another one. It is in some sense implicitly contained in Griewank and Reddien[42].

Lemma 3.3. *Let* $E_0 = \begin{pmatrix} A_0 & B_0 \\ C_0^T & 0 \end{pmatrix} \in \mathbb{R}^{N+p,N+p}$ *be nonsingular and*

let

$$E = \begin{pmatrix} A_0 & B \\ C^T & D \end{pmatrix} \in R^{N+k,N+k}$$ *be another bordering of* A_0. *Solve the*

following $p + k$ *linear systems with* E_0

$$E_0 \begin{pmatrix} X_0 \\ Y_0 \end{pmatrix} = \begin{pmatrix} 0 \\ I_p \end{pmatrix}, \quad E_0 \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} B \\ 0 \end{pmatrix}. \tag{3.14}$$

Then E *is nonsingular iff* Δ *is nonsingular, where*

$$\Delta = \begin{bmatrix} Y & Y_0 \\ C^T X - D & C^T X_0 \end{bmatrix} \in \mathbb{R}^{p+k,p+k}. \tag{3.15}$$

The solution of a system $E \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$ *can be written as*

$$x = x_0 - Xy - X_0 \, d_0 \tag{3.16}$$

where $E_0 \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$ *and* $\Delta \begin{pmatrix} y \\ d_0 \end{pmatrix} = \begin{pmatrix} y \\ C^T x_0 - g \end{pmatrix}$.

The proof is rather easily obtained by inserting the formula (3.16) into the given linear system, and we omit the details. If $k = p$ and $B = B_0$, then we can take $X = 0$, $Y = B_0$. We also notice, that in the extreme case $p = 0$, Lemma 3.3 reduces to the *block elimination method* (e.g. Keller[56]). In the turning point case one might use this Lemma with $B = B_0 = f_\lambda$ and, noticing the coincidence of (3.7) and (3.14), one ends up, for one Newton step, with 2 linear systems in A and one in A^T as well as 2 evaluations of (f_u, f_λ) (see (3.13)). We finally notice that several algorithms have been proposed for solving systems with bordered almost singular matrices as in (3.5). The emphasis here of course is on methods which exploit sparsity of f_u or even work with a black box solver for f_u (see e.g. Rheinboldt[79], Chan[19] and the remarkably simple, recent approach in Govaerts[39]).

5.3.4 Hopf points

We return to the second mechanism of loosing hyperbolicity, i.e., through two complex eigenvalues crossing the imaginary axis. This situation is described by the classical Hopf bifurcation theorem (see e.g. Hassard, Kazarinoff and Wan[46], Amann[3]).

Theorem 3.4. *Let* $(u(\lambda), \lambda)$, *be a smooth stationary branch of (3.1). Assume that at some* $\lambda = \lambda_0$ *the matrix* $f_u^0 = f_u(u(\lambda_0), \lambda_0)$ *has a simple*

eigenvalue $i\omega_0, \omega_0 \neq 0$ with eigenvector $x_0 + iy_0$ and no eigenvalue of the type $ik\omega_0$, $k = 0, 2, 3, \ldots$ Finally, assume

$$Re \; \mu'(\lambda_0) \neq 0, \tag{3.17}$$

where $\mu(\lambda)$ is the continuation of the simple eigenvalue $i\omega_0$ for $f_u(u(\lambda), \lambda)$. Then there exists an $a_0 > 0$ and a smooth branch of $T(a)$-periodic solutions $(u(t, a)(0 \leq t \leq T(a)), \lambda(a)), |a| < a_0$ for $\dot{u} = f(u, \lambda)$ with the following properties

$$u(t, a) = u(\lambda(a)) + a(\cos(\omega_0 t)x_0 - \sin(\omega_0 t)y_0) + \mathcal{O}(a^2)$$
$$\lambda(a) = \lambda_0 + \mathcal{O}(a^2), T(a) = \frac{2\pi}{\omega_0} + \mathcal{O}(a^2). \tag{3.18}$$

Compared to Theorem 3.1, this theorem only describes the geometric setting, i.e., the periodic orbits created out of $(u(\lambda_0), \lambda_0)$ and parametrized by the amplitude a.

For an illustration we now insert a parameter λ into example 1(-) (see 5.1.4).

Example 1(-λ)

$$\dot{x} = y, \; \dot{y} = \lambda - 2y - x^2 + xy. \tag{3.19}$$

As in example 1(λ) the stationary branch is

$$(x(s), y(s), \lambda(s)) = (s, 0, s^2).$$

For the linearization f_u^s at these points we obtain

$$Tr(s) = -2 + s, \; Det(s) = 2s.$$

This is the dotted line shown in Figure 5.3. We have a saddle for $s < 0$, a sink for $0 < s < 2$ and a source for $s > 2$. Consequently, we still find a turning point at $s = 0$, but in addition to this, there is a Hopf bifurcation at $s = 2$. It turns out that the periodic orbits created at $s = 2$ are asymptotically stable and that they exist in a certain interval for $\lambda > 4$. We have sketched the changes in the phase diagram up to this region in Figure 5.11.

In our next step we relate the eigenvalue condition (3.17) of the Hopf Theorem to the regularity of a defining equation. This is the analogy to the equivalence (ii) $\Leftrightarrow$ (iii) in Theorem 3.1.
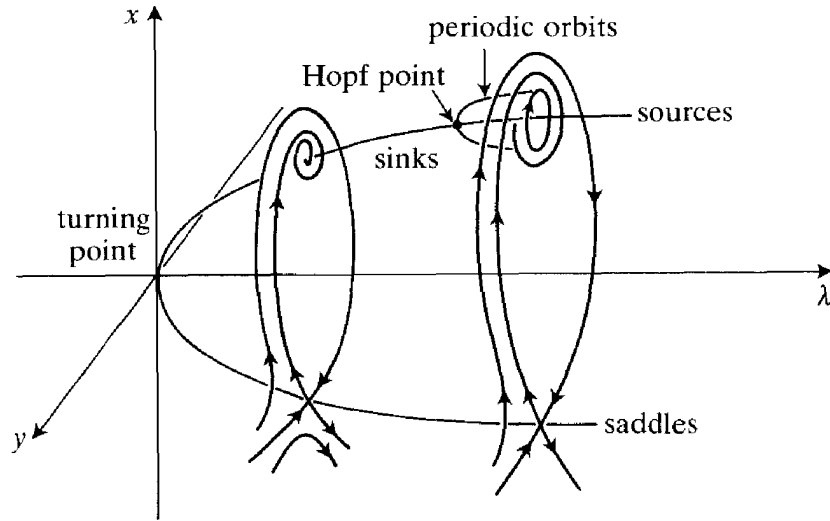
Fig. 5.11. Phase diagrams for Example $1(-\lambda)$

Theorem 3.5. *Let the assumptions of Theorem 3.4 hold with the exception of (3.17) and let $c \in \mathbb{R}^N$ be given such that*

$$c^T x_0 = 0, \quad c^T y_0 = 1.$$

Then the eigenvalue condition (3.17) holds if and only if

$$(u(\lambda_0), \lambda_0, x_0, y_0, \omega_0) \in \mathbb{R}^{3N+2}$$

is a regular solution of the defining equation

$$T(u, \lambda, x, y, \omega) = \begin{pmatrix} f(u, \lambda) \\ f_u(u, \lambda)x + \omega y \\ f_u(u, \lambda)y - \omega x \\ c^T x \\ c^T y - 1 \end{pmatrix} = 0. \qquad (3.20)$$

The system (3.20) was set up and analyzed by Jepson[54]. Further investigations are due to Griewank and Reddien[40], who showed that the linearized system can be reduced to solving several systems with a bordering of $f_u^2(u, \lambda) + \omega^2 I$.

In the spirit of the previous section it seems therefore reasonable to replace (3.20) by the $(N + 2)$-dimensional system

$$T(u, \lambda, \omega) = \begin{pmatrix} f(u, \lambda) \\ g(u, \lambda, \omega) \end{pmatrix} = 0, \qquad (3.21)$$

where $g(u, \lambda, \omega) \in \mathbb{R}^2$ is defined by

$$\begin{pmatrix} f_u^2(u, \lambda) + \omega^2 I & B_0 \\ C_0^T & 0 \end{pmatrix} \begin{pmatrix} v(u, \lambda, \omega) \\ g(u, \lambda, \omega) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{3.22}$$

Since, at the Hopf point $f_u^2 + \omega_0^2 I$ has a two-dimensional null space, spanned by x_0, y_0, it is clear that $B_0, C_0 \in \mathbb{R}^{N,2}$ can be chosen in such a way that (3.22) is nonsingular close to the Hopf-point. Similar strategies, which employ the matrix $f_u^2 + \omega^2 I$ or its characteristic polynomial were proposed by Kubiček and Holodniok[64] and Roose and Hlavacek[83]. Let us consider here one Newton step for (3.20).

As in Lemma 3.2 we solve the adjoint system

$$(W^T G) \begin{pmatrix} f_u^2 + \omega^2 I & B_0 \\ C_0^T & 0 \end{pmatrix} = (0 \ I_2), \quad W \in \mathbb{R}^{N,2}, \ G \in \mathbb{R}^{2,2}$$

and find

$$g = -W^T (f_u^2 + \omega^2 I) v = \quad \text{second column of } G \tag{3.23}$$

$$g_z \zeta = -W^T [f_{uz}(f_u v, \zeta) + f_u \ f_{uz}(v, \zeta)], \quad z = (u, \lambda), \zeta \in \mathbb{R}^{N+1}, \tag{3.24}$$

$$g_\omega = 2\omega \ W^T v. \tag{3.25}$$

Again, g_z can be approximated by difference quotients, and with this information we can set up the bordered matrix

$$T' = \begin{pmatrix} f_u & f_\lambda & 0 \\ g_u & g_\lambda & g_\omega \end{pmatrix}$$

At a Hopf point f_u is regular, so we can solve with T' by a block elimination method. However, as Griewank and Reddien[40] pointed out, turning points are also solutions of (3.20) (and hence of (3.21)), namely with $\omega = 0$. Therefore, one of the algorithms mentioned at the end of the last section is also recommended for this system. Of course, (3.22) requires the computation of f_u^2, but for large banded matrices the computing effort still grows only linearly with N. We should add here, that up to now we have no numerical experience with the system (3.21).

We close this section with some comments on the problem of detecting Hopf points (compare Jepson[54] or Seydel[87] for a discussion). Since the function g in (3.21) is two-dimensional, this problem amounts to watching for a zero of

$$g(u(s), \lambda(s), \omega) \quad \text{at some} \quad \omega \in \mathbb{R}.$$

Clearly, this is a difficult task. One can simply compute all eigenvalues of $f_u(u(s), \lambda(s))$. But then the computational costs usually dominate
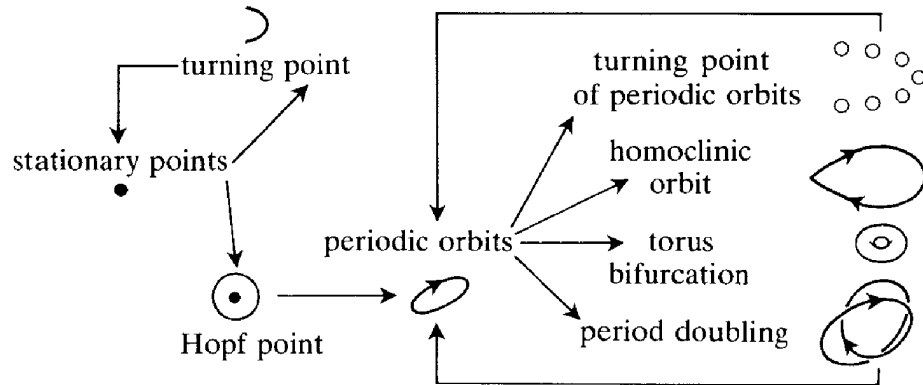
Fig. 5.12.

those for the branch itself, which is particularly awkward for N large and f_u sparse. For a recent attack to this difficult problem by using inserve subspace iteration see Garratt, Moore and Spence[37]. A further possibility for line systems (see 5.1.3, Example 3) is recommended by Seydel[87]. He proposes to use a coarser spatial grid for the Hopf detection.

5.3.5 Singular periodic orbits

Once a branch of periodic orbits has been created at a Hopf point one would like to continue these periodic orbits (cf. 5.2.2) and detect bifurcations on the branch. In Figure 5.12 we have sketched the possible further scenarios by using the list of bifurcations from 5.1.5. We may either find a turning point of periodic orbits, a period doubling, a homoclinic orbit or a torus bifurcation. The last three phenomena already represent final steps on the route to chaotic behaviour, such as a period doubling sequence, periodic forcing of systems with homoclinics and torus breakdown (see Guckenheimer and Holmes[43]).

In what follows, we will focus on only one of the possibilities in Fig. 10, viz. the homoclinic bifurcation.
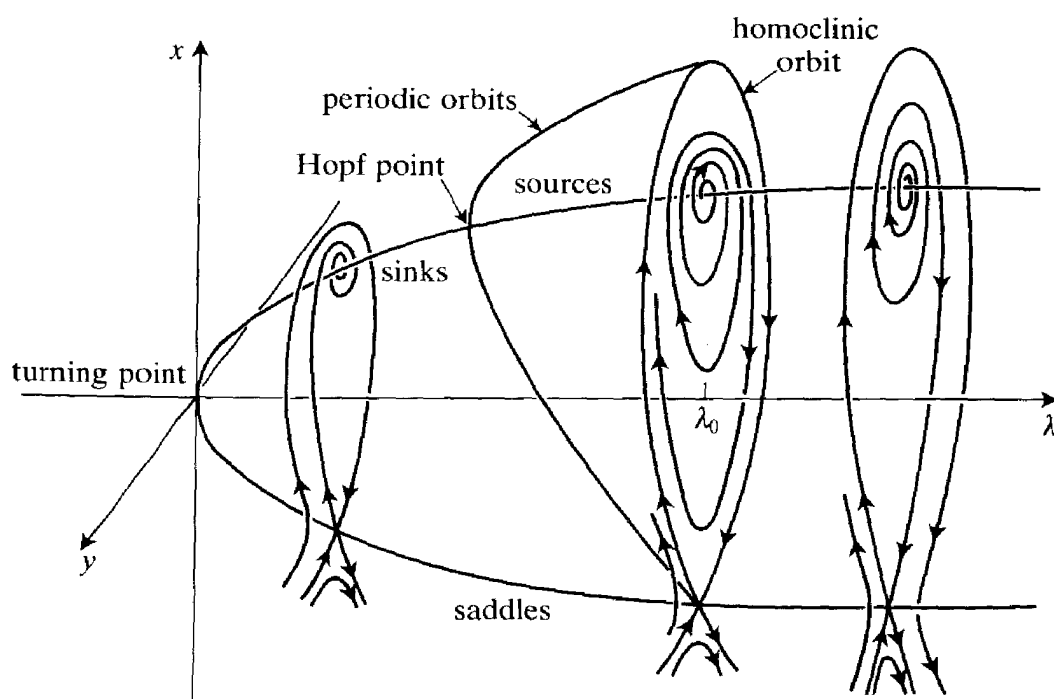
Fig. 5.13. Phase diagram for Example $1(-\lambda)$

5.3.6 The homoclinic bifurcation

Let us continue example $1(-\lambda)$ from section 5.3.4 and observe the fate of the periodic orbit created at the Hopf point. With increasing λ the periods also increase, while the periodic orbits in phase space approach on one side the saddle point. Finally, at some $\lambda = \lambda_0$ the period becomes infinite and the perodic orbit turns into a homoclinic orbit, connecting the unstable saddle with itself in infinite time. Increasing λ beyond λ_0 just leaves us with the two unstable stationary points, and all trajectories not starting at these two points or on their stable manifolds eventually escape to infinity. The phase diagrams are shown schematically in Figure 5.13. Because of the global change of phase diagram at the homoclinic orbit, this transition is often called a *global bifurcation*. Before we can state some basic results we have to introduce further notions. Let $\bar{u}(t), t \in \mathbb{R}$ be a solution of $\dot{u} = f(u, \lambda)$ at some $\lambda = \bar{\lambda}$ such that there exists a $\bar{v} \in \mathbb{R}^N$ with

$$\bar{u}(t) \rightarrow \bar{v} \quad \text{as} \quad t \rightarrow \infty \quad \text{and as} \quad t \rightarrow -\infty. \tag{3.26}$$

Then $\{\bar{u}(t) : t \in \mathbb{R}\}$ is called a *homoclinic orbit* with *base point* $\bar{v}$, and the pair $(\bar{u}, \bar{\lambda})$ is called a *homoclinic orbit pair* (HOP). Obviously, $\bar{v}$ has to be an unstable stationary point of $\dot{u} = f(u, \bar{\lambda})$.

Similar to periodic orbits (see Theorem 2.3) we want to recognize $(\overline{u}, \overline{\lambda})$ as a regular solution of some operator equation. For this purpose, the following Banach spaces are useful.

$$B_0 \;=\; \{u \in C(\mathbb{R}, \mathbb{R}^N) : \lim_{t \to \infty} u(t) \text{ and } \lim_{t \to -\infty} u(t) \text{ exist } \} \qquad (3.27)$$

$$\|u\|_0 \;=\; \sup\; \{\|u(t)\| : t \in \mathbb{R}\} \text{ and} \qquad (3.28)$$

$$B_1 \;=\; \{u \in C^1(\mathbb{R}, \mathbb{R}^N) : u, \dot{u} \in B_0\}, \quad \|u\|_1 = \|u\|_0 + \|\dot{u}\|_0. \qquad (3.29)$$

Next we notice that homoclinic orbits may be phase shifted just as periodic ones (cf. 5.2.2), so for uniqueness we impose a phase condition $\Psi(u) = 0$ where $\Psi : B_0 \to \mathbb{R}$ is assumed to be smooth. We then have the following characterization (see Beyn[11]).

Theorem 3.6. *Let $(\overline{u}, \overline{\lambda})$ be a homoclinic orbit pair with a hyperbolic base point. Then $(\overline{u}, \overline{\lambda}) \in B_1 \times \mathbb{R}$ is a regular solution of the operator equation*

$$F(u, \lambda) = \begin{pmatrix} \dot{u} - f(u, \lambda) \\ \Psi(u) \end{pmatrix} = 0, \quad F : B_1 \times \mathbb{R} \to B_0 \times \mathbb{R} \qquad (3.30)$$

if and only if the following two conditions hold

(i) the only solutions $(v, \mu) \in B_1 \times \mathbb{R}$ of the variational equation

$$\dot{v} = f_u(\overline{u}, \overline{\lambda})v + f_\lambda(\overline{u}, \overline{\lambda})\mu \qquad (3.31)$$

are $v = c\dot{\overline{u}}$ $(c \in \mathbb{R})$, $\mu = 0$.

(ii) $\Psi(\overline{u}) = 0$, $\Psi'(\overline{u})\dot{\overline{u}} \neq 0$.

Remark: Condition (i) is plausible from the fact that $v = c\dot{\overline{u}}$, $\mu = 0$ always solves (3.31), as can be seen by differentiating $\dot{\overline{u}} = f(\overline{u}, \overline{\lambda})$. Moreover, this condition can be characterized by a transversal intersection of certain stable and unstable manifolds (Beyn[12]).

We will not prove Theorem 3.6. However, we would like to draw the reader's attention to an important technical tool which is employed in this as well as the following theorems. The linearization (3.31) suggests that we first have to study the behaviour of linear differential operators

$$Lu = \dot{u} - A(t)u, \quad A(t) \in \mathbb{R}^{N,N} \text{ continuous in } t \in \mathbb{R}.$$

For these, the notion of an *exponential dichotomy* (Coppel[21], Palmer[76]) is of utmost importance. Let $Y(t), t \in \mathbb{R}$ be a fundamental matrix of L normalized by $Y(0) = I$. Then L is said to have an exponential dichotomy

on some interval $J \subset \mathbb{R}$, if there exist $K, \alpha > 0$ and a projection P in $\mathbb{R}^N$ such that for all $t, s \in J$

$$\|Y(t)PY(s)^{-1}\| \leq Ke^{-\alpha(t-s)}, \quad s \leq t \qquad (3.32)$$

$$\|Y(t)(I-P)Y(s)^{-1}\| \leq Ke^{-\alpha(s-t)}, \quad t \leq s. \qquad (3.33)$$

This means that we can decompose the solution operator associated with L into a part which decays exponentially in forward time and another part which decays exponentially in backward time. This property holds for the linear differential operator L obtained by setting

$$A(t) = f_u(\overline{u}(t), \overline{\lambda}),$$

where $(\overline{u}, \overline{\lambda})$ is the HOP. Using the hyperbolicity of the base point, one can show that L has an exponential dichotomy on both $J = [0, \infty)$ and $J = (-\infty, 0]$ (but not on $J = \mathbb{R}!$). These dichotomies may then be used to set up a linear Fredholm theory for the operator $L : B_1 \to B_0$. In fact, in our homoclinic case L turns out to have Fredholm index zero.

Theorem 3.6 gives rise to the following definition. A HOP $(\overline{u}, \overline{\lambda})$ is called *nondegenerate*, if the base point is hyperbolic and if condition (i) of Theorem 3.6 holds (see Beyn[11] for the general case of connecting orbits). It is remarkable that this basic assumption suffices to guarantee a branch of periodic orbits created out of the homoclinic orbit according to the following *homoclinic bifurcation theorem*.

Theorem 3.7. *Let $(\overline{u}, \overline{\lambda})$ be a nondegenerate homoclinic orbit pair of*

$$\dot{u} = f(u, \lambda). \qquad (3.34)$$

Then there exists a $T_0 > 0$ and a branch of $2T$-periodic solutions

$$(u(t, T)(|t| \leq T), \lambda_T), \quad T \geq T_0$$

of the system (3.34) with the following estimates

$$\|\overline{u}(t) - u(t, T)\| \leq C e^{-\alpha T} \quad \text{for all } t \in [-T, T]$$
$$|\overline{\lambda} - \lambda_T| \leq C e^{-2\alpha T} \qquad (3.35)$$

where $\alpha < |Re\,\mu|$ for all eigenvalues μ of the linearization at the base point.

Surprisingly, this general theorem seems not to have been noticed until recently (Lin[69], Beyn[12]), although there is a long history of homoclinic bifurcation results (cf. Andronov, Leontovich, Gordon and Maier[4], Chow and Hale[20], Guckenheimer and Holmes[43], Wiggins[100]). One reason may be that the cited references try to discuss simultaneously the dynamics
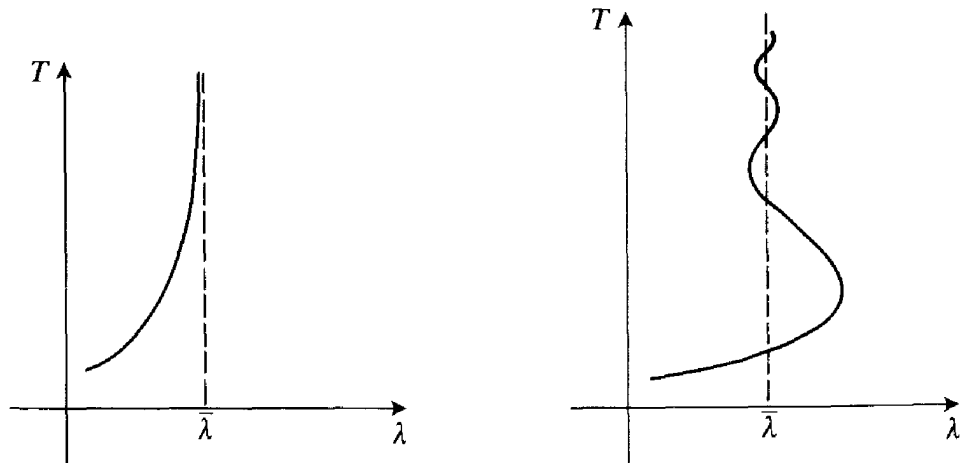
Fig. 5.14. Typical diagrams at a homoclinic bifurcation

of (3.34) for λ close to $\bar{\lambda}$. However, these can be very complicated in dimensions $N \geq 3$. In Figure 5.14 we sketch two basic behaviours of the periodic branch in a (λ, T) diagram. Let us denote those eigenvalues at the hyperbolic base point as *critical* which have smallest positive or largest negative real part. Then case 1 in Figure 5.14 usually occurs when the two critical eigenvalues are real, while in case 2 there is a real and a complex conjugate pair of critical eigenvalues. This last case is called the Shil'nikov bifurcation, see Shil'nikov[88], Glendinning,[38], Wiggins[100], Lin[69]. One of its remarkable features is that there exist infinitely many periodic orbits at $\lambda = \bar{\lambda}$.

Theorem 3.7 also has an impact on numerical calculations. It shows that HOP's may well be approximated by periodic orbits of large but fixed periods, and this approach has been successfully used by Doedel and Kernevez[28].

However, it is possible to replace the periodic boundary conditions by more efficient ones, the so-called *projection boundary conditions*, which lead to even better convergence than (3.35) and hence allow for smaller time intervals. We will briefly discuss here the method of Beyn[11,12], and we mention that a slightly different method was developed by Doedel and Friedman[29,30] (see also Kuznetsov[67], Rodrigues-Luis, Freire and Ponce[81]). Both approaches allow for the computation of more general *connecting orbits*, i.e., orbits which connect two possibly different stationary points.

We know from Theorem 3.6 that we have to solve a defining equation, which is a parametrized boundary value problem on the real line

$$\dot{u} = f(u, \lambda), \quad u \in B_1, \lambda \in \mathbb{R}, \tag{3.36}$$

$$\Psi(u) = 0. \tag{3.37}$$

For numerical purposes we have to truncate this boundary value problem to a finite interval $J = [T_-, T_+]$, and we have to set up boundary conditions at T_-, T_+ which catch the asymptotic behaviour of the solution (notice that in (3.36) the boundary conditions are hidden in the space B_1). For the case of semi-infinite intervals such boundary conditions have been set up by de Hoog and Weiss[22] and Lentini and Keller[68]. Here we generalize the first approach to our problem (3.36).

We require that a branch of stationary hyperbolic points $v(\lambda)$, is known (or can at least be computed numerically) which contains the candidates for the base points (compare Figure 5.13). Consider the *stable subspace* $Y_s(\lambda)$ of $f_u(v(\lambda), \lambda)$, which contains all generalized eigenvectors belonging to the eigenvalues with negative real part, and similarly let $Y_u(\lambda)$ be the *unstable subspace*. Then we impose the projection boundary conditions

$$u(T_+) - v(\lambda) \in Y_s(\lambda), \quad u(T_-) - v(\lambda) \in Y_u(\lambda). \tag{3.38}$$

These conditions are very natural since the homoclinic orbit must leave $v(\lambda)$ via its unstable manifold, which is tangent to $Y_u(\lambda)$, and must approach $v(\lambda)$ again via its stable manifold, which is tangent to $Y_s(\lambda)$ (see Figure 5.15 and, for example, Irwin[51]). For a numerical implementation we construct full rank matrices

$$P_s(\lambda) \in \mathbb{R}^{N_u, N}, \quad P_u(\lambda) \in \mathbb{R}^{N_s, N}, \quad N_u = N - N_s$$

such that

$$Y_s(\lambda) = \{z : P_s(\lambda)z = 0\}, \quad Y_u(\lambda) = \{z : P_u(\lambda)z = 0\}$$

and rewrite (3.38) as

$$P_s(\lambda)(u(T_+) - v(\lambda)) = 0, \quad P_u(\lambda)(u(T_-) - v(\lambda)) = 0. \tag{3.39}$$

These projection type matrices can be computed numerically in such a way that the smooth dependence on λ is guaranteed (see Beyn[11]).

Finally, bearing in mind the discussion of phase conditions in 5.2.2, we replace (3.37) by an integral condition

$$\Psi_I(u) = \int_{T_-}^{T_+} z_0^T(t)(u(t) - u_0(t)) \, dt = 0, \tag{3.40}$$
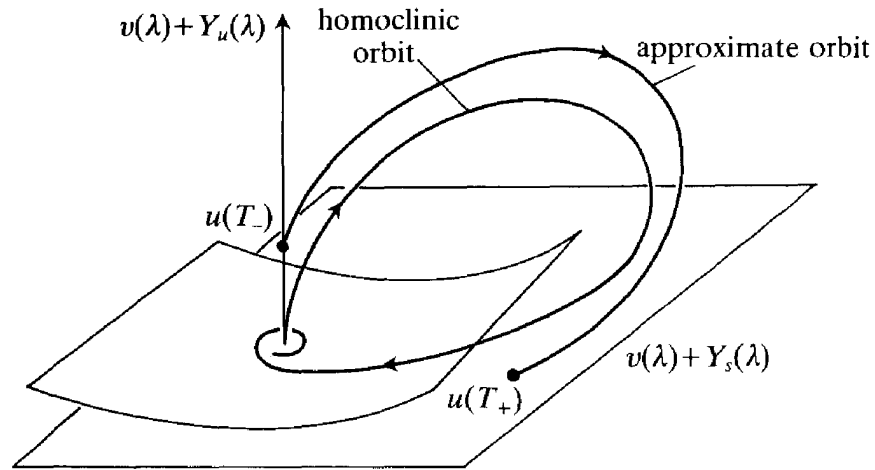
Fig. 5.15. Illustration of projection boundary conditions

where $u_0(t)$ is some initial approximation and $z_0(t) \approx \dot{u}_0(t)$. Summing up, we have to solve the $(N+1)$-dimensional system

$$\dot{u} = f(u, \lambda), \quad \dot{\lambda} = 0 \quad \text{for} \quad t \in [T_-, T_+] \tag{3.41}$$

subject to the $N + 1$ boundary conditions (3.39), (3.40). Notice that (3.39) is linear in u but nonlinear in λ.

As in Theorem 3.7 the approximation error, due to the truncation to the finite interval, can be estimated for $[T_-, T_+]$ sufficiently large (see Beyn[11, 12]).

Theorem 3.8. *Let* $(\bar{u}, \bar{\lambda})$ *be a nondegenerate homoclinic orbit pair and assume that in the phase condition (3.40) we use functions* $z_0, u_0 \in B_0$ *such that*

$$\int_{-\infty}^{+\infty} z_0^T(t)(\bar{u}(t) - u_0(t))\, dt = 0, \quad \int_{-\infty}^{\infty} z_0^T(t)\dot{\bar{u}}(t)\, dt \neq 0. \tag{3.42}$$

Then there exists a $T_0 > 0$, *such that for* $T_+, -T_- \geq T_0$ *the boundary value problem (3.39)–(3.41) has a unique solution* $(u_{[T_-,T_+]}, \lambda_{[T_-,T_+]})$ *close to* $(\bar{u}|_{[T_-,T_+]}, \bar{\lambda})$ *and the following estimates hold for a suitable phase shift* $\tau = \tau(T_-, T_+)$

$$\|\bar{u}(t + \tau) - u_{[T_-,T_+]}(t)\| \leq C\, e^{-2\alpha\, \text{Min}(|T_-|, T_+)}, \quad t \in [T_-, T_+]$$

$$|\bar{\lambda} - \lambda_{[T_-,T_+]}| \leq C\, e^{-3\alpha\, \text{Min}(|T_-|, T_+)} \tag{3.43}$$

where α *is a given constant with* $\alpha < |Re\, \mu|$ *for all eigenvalues* μ *of the linearization at the base point.*

The requirements for the phase fixing of the continuous homoclinic orbit are not really restrictive, since we are only interested in approximating it up to a phase shift. We notice that (3.43) has better exponents that (3.35) and this difference can be clearly seen in practical computations. Also, for both types of boundary conditions we have a superconvergence phenomenon in the parameter. This also shows up numerically, and in some cases the λ-error is even smaller than the prediction from (3.43).

We consider as a final example the Lorenz equations (cf. Sparrow[90]).

Example 5

$$\dot{x} = \sigma(y - x), \quad \dot{y} = \lambda\, x - y - xz, \quad \dot{z} = -\mu z + xy.$$

First, at the Lorenz values $\sigma = 10$, $\mu = \frac{8}{3}$ the homoclinic orbit connecting the origin with itself and the λ-value ($= 13.926557$) were computed. Due to the symmetry in the Lorenz equation this homoclinic orbit has a symmetric companion orbit, and both together create a strange invariant set (see Sparrow[90], Glendinning[38]) which at higher λ-values stabilizes to an attractor.

We then continued this HOP into a branch of HOP's by freeing the parameter μ. In addition, the automatic adaptation strategy for $[T_-, T_+]$, as developed in Beyn[11], was used. Some of the homoclinic orbits from this branch are shown in an xy-projection in Figure 5.16.

5.4 Two–parameter problems

In this chapter we discuss some aspects of two–parameter systems

$$\dot{u} = f(u, \lambda), \quad \lambda = (\lambda_1, \lambda_2) \in \mathbb{R}^2, \quad u(t) \in \mathbb{R}^N. \tag{4.1}$$

It is evident that in such systems singular points with higher degeneracies are possible, and one might well ask why one should analyze or even numerically compute these points. The answer is that these singular points serve as *organizing centers* for dynamic features, which are obtained under parametric perturbations. And these dynamic features may well be generic, i.e., they appear in 0-parameter problems (e.g., invariant tori), and so we may start a branch of these objects at the singularity. In addition, from two-parameter problems onwards, chaotic behaviour is possible near singularities, so that there is some chance for an analytical treatment. This is one of the important discoveries of dynamical systems theory.
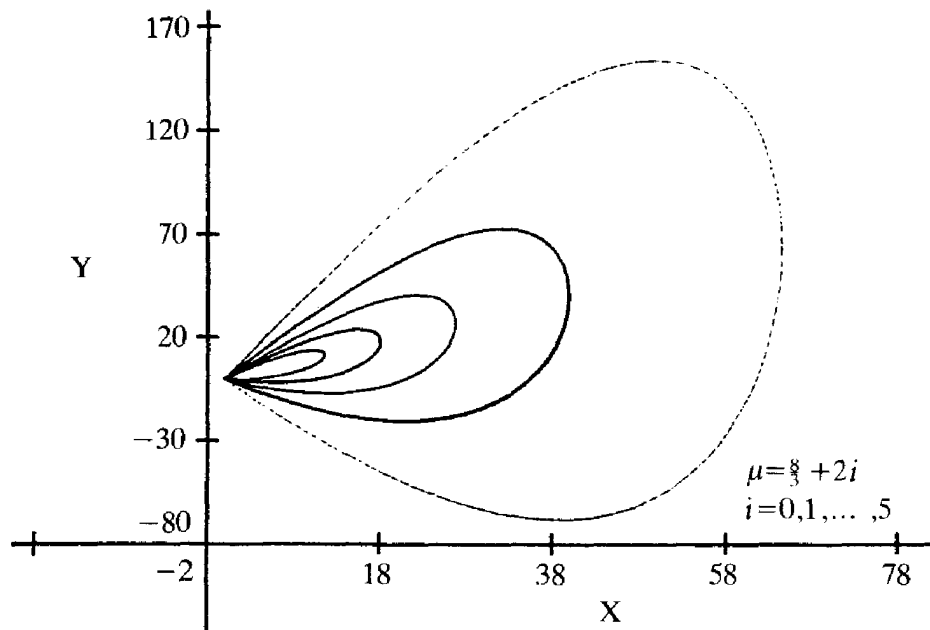
Fig. 5.16. Some homoclinic orbits of the Lorenz equations

5.4.1 The possibilities

Suppose that we continue a branch of stationary points $(u(s), \lambda(s))$, $s \in \mathbb{R}$ of (4.1) which are singular (u, λ_1)-points, i.e., either a branch of Hopf points or turning points. Thus the Jordan normal form J^s of $f_u^s = f_u(u(s), \lambda(s))$ is of the type

$$J^s = \begin{pmatrix} 0 & 0 \\ 0 & H(s) \end{pmatrix} \quad \text{or} \quad J^s = \begin{bmatrix} 0 & \omega(s) & 0 \\ -\omega(s) & 0 & 0 \\ 0 & 0 & H(s) \end{bmatrix}$$

For most of the points we expect the submatrix $H(s)$ to be hyperbolic, but at some values of s it may be nonhyperbolic. However, the reader is cautioned that the Jordan structure (along with some nondegeneracy conditions for quadratic terms) is no longer sufficient for classifying the singularities in two-parameter problems. For example, on a branch of turning points we may find a degeneracy in the quadratic terms, viz.(compare (3.3)),

$$f_{uu}^s \, \phi_s^2 \in R(f_u^s),$$

where ϕ_s spans the null space of f_u^s. This is the well-known *cusp point* (see Guckenheimer and Holmes[43], Chapter 7.1 and for numerical methods Spence and Werner[91], Roose and Piessens[84], Pönisch[77], Griewank and Reddien[42]). For the remaining three possibilities we have a singular block

in the Jordan form of one of the following types

$$
\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad
\begin{pmatrix} 0 & \omega & 0 \\ -\omega & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad
\begin{pmatrix} 0 & \omega_1 & 0 & 0 \\ -\omega_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega_2 \\ 0 & 0 & -\omega_2 & 0 \end{pmatrix}. \tag{4.2}
$$

The analysis of the first case is generally attributed to Bogdanov[15] and Takens[97]. Consequently, we call these points *Takens-Bogdanov singularities* or *TB-points*. A numerical method for computing TB-points was given by Roose[82]; see also Khibnik[59] and the further references therein. Here we will pursue the corresponding defining equation from the viewpoint taken in section 5.3, i.e. we will follow Griewank and Reddien[42]. It will become clear from the following presentation and from the treatment of Hopf points in 5.3.4, how to construct defining equations for the remaining cases in (4.2). We notice that these bifurcations can only occur in systems of dimensions $N \geq 3$ and $N \geq 4$ and a complete analysis of these cases is still not available, mainly due to the local occurrence of chaotic behaviour (Guckenheimer and Holmes[43]).

5.4.2 The Takens-Bogdanov singularity

Let us first consider a two-dimensional example which contains all the variations of example 1 (see 5.1.3, 5.1.4, 5.3.2, 5.3.4, 5.3.6).

Example 1(λ_1, λ_2)

$$
\dot{x} = y, \quad \dot{y} = \lambda_1 + \lambda_2 y - x^2 + xy. \tag{4.3}
$$

In 5.3.2, 5.3.4, 5.3.6 we studied the cases $\lambda_2 = 1$ and $\lambda_2 = -2$ with varying λ_1. In the general case of (4.3) the stationary points lie on the folded surface

$$
S = \{(x, y, \lambda_1, \lambda_2) = (s, 0, s^2, \lambda_2) : s, \lambda_2 \in \mathbb{R}\}
$$

and the trace and determinant of f_u at an arbitrary point on S are given by

$$
\text{Tr}(s, \lambda_2) = \lambda_2 + s, \quad \text{Det}(s, \lambda_2) = 2s.
$$

Varying s and λ_2, these values now cover the whole plane in Figure 5.3. Hopf bifurcation occurs on the half-parabola

$$
\lambda_2 = -s, \lambda_1 = s^2, \quad s > 0. \tag{4.4}
$$

The periodic orbits created at these Hopf points vanish through a homoclinic orbit on a curve which in a neighbourhood of $\lambda_1 = \lambda_2 = 0$ is approximately given by

$$
\lambda_1 = \left(\frac{7}{5}\lambda_2\right)^2, \quad \lambda_2 < 0.
$$

System (4.3) is in fact a so-called *unfolding* of the system

$$\dot{x} = y, \quad \dot{y} = -x^2 + xy,$$

which has 0 as a TB-point (see Guckenheimer and Holmes[43], Chapter 7 and notice that we slightly transformed the system). The qualitative information on the various phase diagrams is contained in Figure 5.17.

For the numerical computation of a TB-point let us start as in (4.1) with a branch of λ_1-turning points $(u(s), \lambda(s))$, obtained by solving

$$T(u, \lambda) = \left(\begin{array}{c} f(u, \lambda) \\ g(u, \lambda) \end{array} \right) = 0,$$

where

$$A(u, \lambda) \left(\begin{array}{c} v(u, \lambda) \\ g(u, \lambda) \end{array} \right) = \left(\begin{array}{c} 0 \\ 1 \end{array} \right), \quad A(u, \lambda) = \left(\begin{array}{cc} f_u(u, \lambda) & b_0 \\ c_0^T & 0 \end{array} \right) \qquad (4.5)$$

and

$$(\Psi^T(u, \lambda), g(u, \lambda)) \, A(u, \lambda) = (0, 1). \qquad (4.6)$$

Compare with (3.6), but notice that now $\lambda \in \mathbb{R}^2$.

A test function for detecting a TB-point is then (cf. Roose[82], Spence, Cliffe and Jepson[92])

$$\tau(s) = \Psi^T(u(s), \lambda(s)) \, v(u(s), \lambda(s)), \qquad (4.7)$$

because we expect the left eigenvector of f_u to be orthogonal to the right eigenvector at a TB-point.

For the accurate location of the TB-point we now set up the defining system

$$S(u, \lambda) = \left(\begin{array}{c} f(u, \lambda) \\ g(u, \lambda) \\ h(u, \lambda) \end{array} \right) = 0 \qquad (4.8)$$

where $h(u, \lambda)$ is defined by

$$A(u, \lambda) \left(\begin{array}{c} w(u, \lambda) \\ h(u, \lambda) \end{array} \right) = \left(\begin{array}{c} v(u, \lambda) \\ 0 \end{array} \right). \qquad (4.9)$$

It is also natural to solve the adjoint system

$$(\zeta^T(u, \lambda), \tilde{h}(u, \lambda)) \, A(u, \lambda) = (\Psi^T(u, \lambda), 0). \qquad (4.10)$$

By similar manipulations as in the proof of Lemma 3.2, we then obtain the following result (see Griewank and Reddien[42]).
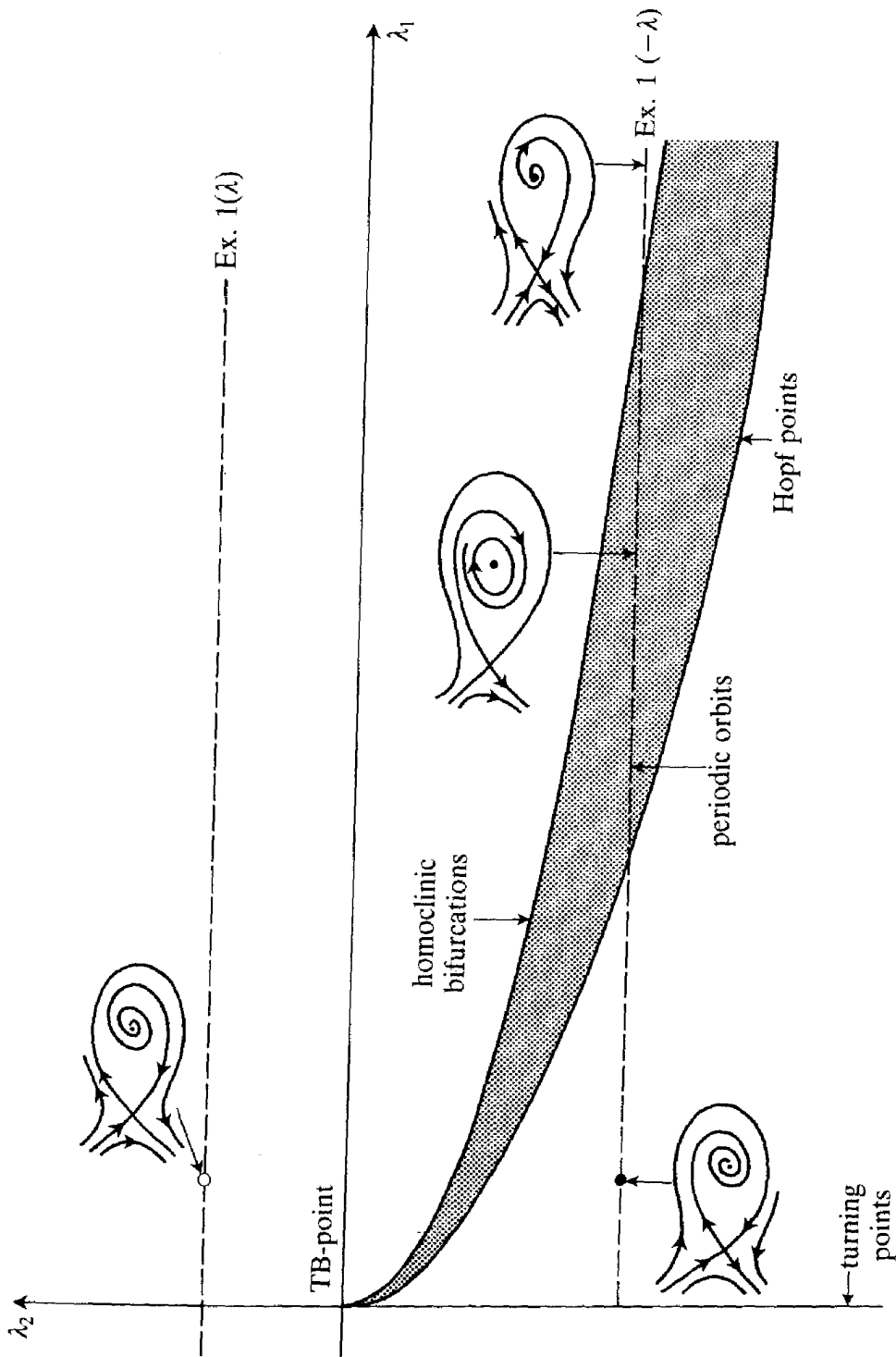
Fig. 5.17. Unfolding picture at a TB-point

Lemma 4.1. *For any* (u, λ), *where* $A(u, \lambda)$ *is nonsingular, the functions defined in (4.5), (4.6) and (4.9), (4.10) satisfy the following relations*

$$h = \tilde{h} = \Psi^T v \tag{4.11}$$

$$h_z = -\Psi^T f_{uz} w - \zeta^T f_{uz} v, \quad z = (u, \lambda). \tag{4.12}$$

From this we see that the test function in (4.7) is in fact obtained by evaluating h along the branch. Though this could have been done without solving (4.9), (4.10), we find from (4.12) that the derivatives of h can be easily expressed in terms of those solutions (using a difference formula for the second derivative of f, if necessary). Thus we can evaluate the Jacobian

$$S' = \begin{pmatrix} f_u & f_\lambda \\ g_u & g_\lambda \\ h_u & h_\lambda \end{pmatrix}$$

and we may now solve for the Newton step by invoking Lemma 3.3 with $p = 1$ and $k = 2$.

A careful count of the numerical work for one Newton step (notice the coincidence of (4.5) with the first system in (3.14)) yields 5 linear systems in A, two in A^T and 4 evaluations of (f_u, f_λ).

Similar to Roose[82] the regularity of (4.8) at some solution can be related to a nonvanishing derivative of the test function (4.7) under further assumptions. We don't discuss any details here. Instead, let us write down the various functions above for the simple example 1 (λ_1, λ_2). With $u = (x, y)$, $b_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $c_0^T = (1, 0)$ we find

$$v(u, \lambda) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad g(u, \lambda) = 2x - y,$$

$$\Psi^T(u, \lambda) = (-\lambda_2 - x, 1), \quad h(u, \lambda) = -\lambda_2 - x$$

and thus

$$S'(u, \lambda) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -2x + y & \lambda_2 + x & 1 & y \\ 2 & -1 & 0 & 0 \\ -1 & 0 & 0 & -1 \end{pmatrix},$$

and

$$S'(0, 0) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 2 & -1 & 0 & 0 \\ -1 & 0 & 0 & -1 \end{pmatrix}.$$

Clearly, $S'(0, 0)$ is nonsingular.

5.4.3 Starting 1-parameter singularities at a TB-point

In the last section we discussed the passage from a branch of 1-parameter singularities to a 2-parameter singularity. If we think of the singularities being ordered in a hierarchy, then we may call this step '*descending the hierarchy*', a term coined by Jepson and Spence[55] for stationary problems. See also the hierarchy described by Khibnik[59]. Of equal importance is the reverse step of *ascending the hierarchy*, i.e., starting a branch of 1-parameter singularities from a 2-parameter singularity. In fact, the calculation of TB-points was taken up by Roose[82] in order to start branches of Hopf-points (see also Spence, Cliffe and Jepson[92]).

If we look at the unfolding picture Figure 5.17, then this suggests to try starting a branch of homoclinic orbits at a TB-point. This was first carried out for planar systems with the help of Melnikov's method by Freire, Ponce and Rodriguez-Luis[36], see also Rodriguez-Luis, Freire and Ponce[81]. We will briefly outline here the algorithm for the general case (more details are contained in Beyn[13]). Though this algorithm involves several steps, it is not very difficult to implement. Its derivation, however, needs all the theoretical machinery developed for proving the existence of a branch of homoclinic orbits, such as *center manifolds*, *normal forms* and *Melnikov's method*.

We assume, that we have computed a TB-point $(u_0, \lambda_0) \in \mathbb{R}^{N+2}$ as in the last section, and we will use the matrix $A_0 = A(u_0, \lambda_0)$ as well as the (generalized) right and left eigenvectors v, w and Ψ, ζ of f_u^0 (see (4.5), (4.6), (4.9), (4.10)). We also assume that these vectors are normalized such that

$$\zeta^T v = \Psi^T w = 1, \quad \Psi^T v = \zeta^T w = 0. \tag{4.13}$$

This can always be achieved by replacing Ψ, ζ by $\alpha\Psi$, $\alpha\zeta + \beta\Psi$ for some suitable α, β. Finally, we require $\Psi^T f_\lambda^0 \neq 0$ and without loss of generality we can assume

$$\delta = \Psi^T f_{\lambda_1}^0 \neq 0. \tag{4.14}$$

Otherwise, we exchange the roles of λ_1 and λ_2. We then proceed as follows:

Step 1 Linear normal form:

Introduce new coordinates $z \in \mathbb{R}^N$, $\mu \in \mathbb{R}^2$ via a linear transformation

$$\begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} u_0 \\ \lambda_0 \end{pmatrix} + \begin{pmatrix} R & v & w & D_1 & D_2 \\ 0 & 0 & 0 & B_1 & B_2 \end{pmatrix} \begin{pmatrix} z \\ \mu \end{pmatrix}, \tag{4.15}$$

with $R \in \mathbb{R}^{N,N-2}$, $D_1, D_2 \in \mathbb{R}^N$, $B_1, B_2 \in \mathbb{R}^2$, such that the system $\dot{u} = f(u, \lambda)$ takes the form

$$\dot{z} = g(z, \mu) \tag{4.16}$$

with

$$g_z(0,0) = \begin{bmatrix} H & 0 \\ 0 & J \end{bmatrix}, \quad g_\mu(0,0) = \begin{bmatrix} 0 \\ J^T \end{bmatrix},$$

and

$$H \in \mathbb{R}^{N-2,N-2} \text{ hyperbolic}, \quad J = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

This form is obtained by setting

$$B_1 = \begin{pmatrix} B_{11} \\ 0 \end{pmatrix} = \begin{pmatrix} \delta^{-1} \\ 0 \end{pmatrix}, \quad B_2 = \begin{pmatrix} B_{12} \\ 1 \end{pmatrix} = \begin{pmatrix} -\delta^{-1}\Psi^T f^0_{\lambda_2} \\ 1 \end{pmatrix}$$

and by solving the two linear systems

$$A_0 \begin{pmatrix} D_1 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} \zeta - B_{11} f^0_{\lambda_1} \\ 0 \end{pmatrix}, \quad A_0 \begin{pmatrix} D_2 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} -B_{12} f^0_{\lambda_1} - f^0_{\lambda_2} \\ 0 \end{pmatrix}.$$

$$(4.17)$$

Step 2   Center manifold reduction:

Write $z = (\eta, \xi) \in \mathbb{R}^{N-2} \times \mathbb{R}^2$, then there are locally invariant two-dimensional center manifolds which are graphs of the type $\eta = F(\xi, \mu)$. Inside the manifolds the system (4.16) reduces to

$$\dot{\xi} = \begin{pmatrix} g_{N-1} \\ g_N \end{pmatrix} (F(\xi, \mu), \xi, \mu) =: h(\xi, \mu).$$

$$(4.18)$$

Furthermore, h has a Taylor expansion

$$h(\xi, \mu) = \begin{pmatrix} \xi_2 \\ \mu_1 \end{pmatrix} + Q(\xi, \mu) + \mathcal{O}((\|\xi\| + \|\mu\|)^3),$$

where Q contains the quadratic terms. Only the following ones are needed for our further calculation

$$Q(\xi, \mu) = \begin{pmatrix} p_{11}\xi_1^2 + p_{14}\xi_1\mu_2 + \dots \\ q_{11}\xi_1^2 + q_{12}\xi_1\xi_2 + q_{14}\xi_1\mu_2 + q_{24}\xi_2\mu_2 + q_{44}\mu_2^2 + \dots \end{pmatrix},$$

and these are given by

$$\begin{aligned}
p_{11} &= \zeta^T f^0_{uu} v^2, \\
p_{14} &= \zeta^T (f^0_{uu} v D_2 + f^0_{u\lambda} v B_2) \\
q_{11} &= \Psi^T f^0_{uu} v^2, \quad q_{12} = \Psi^T f^0_{uu} vw \\
q_{14} &= \Psi^T (f^0_{uu} v D_2 + f^0_{u\lambda} v B_2) \\
q_{24} &= \Psi^T (f^0_{uu} w D_2 + f^0_{u\lambda} w B_2) \\
q_{44} &= \Psi^T (f^0_{uu} D_2^2 + 2 f^0_{u\lambda} D_2 B_2 + f^0_{\lambda\lambda} B_2^2).
\end{aligned}$$

Usually, the next step consists in a normal form transformation of the quadratic terms. However, we omit this step, since many of the quadratic terms prove to be irrelevant after the following scaling transformation.

Step 3 Scaling transformation:

Again new coordinates are introduced

$$(\xi_1, \xi_2) \rightarrow (x, y), \quad (\mu_1, \mu_2) \rightarrow (\epsilon, \tau)$$

such that the two dimensional system (4.17) assumes the form

$$
\begin{aligned}
\dot{x} &= y + \epsilon(a_1 x^2 + a_2 \tau x + a_3 \tau^2) + \mathcal{O}(\epsilon^2) \\
\dot{y} &= x^2 - 4 + \epsilon(b_1 xy + b_2 \tau y) + \mathcal{O}(\epsilon^2)
\end{aligned}
\qquad (4.19)
$$

The transformation is of the form

$$
\begin{aligned}
\mu_1 &= (\alpha_0 + \alpha_1 \tau^2)\epsilon^4, \quad \mu_2 = \tau\epsilon \\
\xi_1(t) &= \alpha_2 \epsilon^2 (x(\alpha_3 \epsilon t) + \alpha_4 \tau) \\
\xi_2(t) &= \alpha_5 \epsilon^3 y(\alpha_3 \epsilon t).
\end{aligned}
$$

The constants α_i, $i = 0, \ldots, 5$ are determined in such a way that the special system (4.19) is obtained.

The coefficients a_i and b_j can be explicitly expressed in terms of the quadratic coefficients from the last step. But we don't write down these relations because a complete set of formulas for an approximate homoclinic orbit of (4.17) will be given below.

Step 4 Melnikov's method:

First notice that the unperturbed system (4.19) ($\epsilon = 0$) is Hamiltonian and has the homoclinic orbit

$$(\bar{x}(t), \bar{y}(t)) = 2(1 - 3\text{sech}^2(t), \ 6\text{sech}^2(t)\tanh(t)).$$

Melnikov's method (Melnikov[71], Guckenheimer and Holmes[43]) can now be used to show how this homoclinic orbit survives for $\epsilon \neq 0$. Instead of the above two references we strongly recommend Hale's reformulation of Melnikov's method as a problem of bifurcation from the trivial solution (Hale[45]). In fact, taking τ as the bifurcation parameter, we see that $(\bar{x}, \bar{y}, \epsilon = 0)$ is a trivial branch of HOP's for (4.19). After some analysis, which employs the techniques from 5.3.6, we then find that bifurcation from a simple eigenvalue occurs at

$$\tau_0 = \frac{10}{7} \frac{2a_1 + b_1}{a_2 + b_2}.$$

Taking the last two steps together, we find an approximate homoclinic orbit for (4.17) by choosing some small ϵ and setting
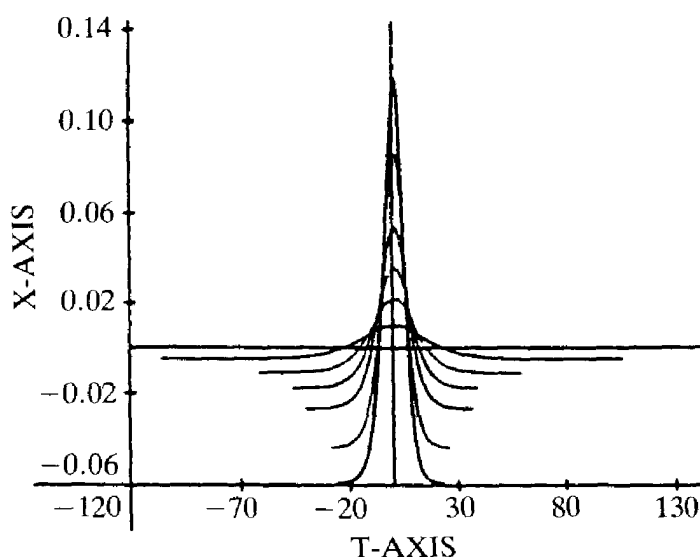
Fig. 5.18. Homoclinic orbits starting at a TB-point: the time diagram, $\lambda_1 = 0.25 \cdot 10^{-4}, \ldots, 0.35 \cdot 10^{-2}$.

$$\mu_1 = \sigma_0 \epsilon^4, \quad \mu_2 = \tau_0 \epsilon^2,$$

$$\xi_1(t) = \frac{\epsilon^2}{q_{11}} \left(1 - 3 \operatorname{sech}^2\left(\frac{\epsilon}{2} t\right) - q_{14}\tau_0\right)$$

$$\xi_2(t) = \frac{3\epsilon^3}{q_{11}} \operatorname{sech}^2\left(\frac{\epsilon}{2} t\right) \tanh\left(\frac{\epsilon}{2} t\right),$$

where

$$\tau_0 = \frac{5}{7} \frac{p_{11} + q_{12}}{q_{11}p_{14} - p_{11}q_{14} + q_{24}q_{11} - q_{14}q_{12}}, \quad \sigma_0 = \frac{1}{2q_{11}} \left((q_{14}^2 - q_{11}q_{44})\tau_0^2 - 1\right)$$

$$(4.20)$$

Of course, we require the two denominators in (4.20) to be nonzero. These are the crucial conditions which in conjunction with the assumptions on f_u^0 define a *nondegenerate TB-point*. For our model example (4.3) they are satisfied because the coefficients in front of x^2 and xy do not vanish.

The above formulae can finally be used to set up an approximate homoclinic orbit for the original problem via

$$\widetilde{u}(t) = \xi_1(t)v + \xi_2(t)w + D_1\mu_1 + D_2\mu_2 + u_0$$

$$\widetilde{\lambda} = \mu_1 B_1 + \mu_2 B_2 + \lambda_0 \quad \text{(cf. step 1)}.$$

With this approximation we can employ the numerical method for homoclinic orbit pairs from (3.6). In the beginning we look for a HOP (u, λ_2) close to $(\widetilde{u}, \widetilde{\lambda}_2)$ with $\lambda_1 = \widetilde{\lambda}_1$ fixed. Then λ_1 is freed and used for continuation. This approach has been tried successfully on a series of examples.
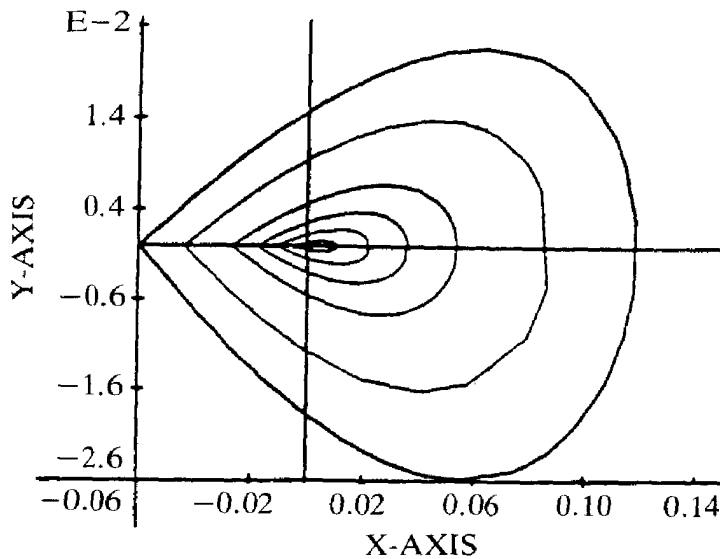
Fig. 5.19. Homoclinic orbits starting at a TB-point: the phase diagram, $\lambda_1 = 0.25 \cdot 10^{-4}, \ldots, 0.35 \cdot 10^{-2}$.

However, sometimes difficulties arise with the realization of the projection boundary conditions since we are very close to the fold of the stationary surface (cf. 5.4.2). We display in Figures 5.18 and 5.19 some results for our model example (5.4.3). The computation was started with $\epsilon = 0.1$ and then continuation with respect to λ_1 and the automatic truncation strategy was used (cf. Figure 5.16).

5.5 The longtime behaviour of integration methods

5.5.1 Comparison of discrete and continuous flows

In section 5.1.2 we already considered the basic problems, which occur when comparing the longtime dynamics of a one-step method with that of the dynamical system. Of course, in practice one would prefer to use a sophisticated code (variable step size, variable order) for the initial value problem

$$\dot{u} = f(u), \quad u(0) = u^0 \in \mathbb{R}^N. \tag{5.1}$$

The user prescribed tolerances of these codes however, can only control the local discretization error, and in principle there is no escape from the exponential growth of the global error as signalled by the estimate (1.8). It may occur just at a later time than with a simple minded one-step method. Whether this blow-up of the error really occurs, clearly depends on the dynamics of the system (5.1) itself. In what follows we will focus on

the behaviour of the sequence

$$u^{n+1} = \phi(h, u^n), \ n = 0, 1, 2, \ldots, \ u^0 \in \mathbb{R}^N, \tag{5.2}$$

if n tends to infinity, but h is sufficiently small (this simulates the accurate ordinary differential equation-solver). For line systems of partial differential equations, even this may be an unrealistic situation.

We start with a discussion of the relations between the discrete h-flow $\phi(h, \cdot)$ and the continuous h-flow $\Phi(h, \cdot)$. For an illustration we use *m-stage explicit Runge-Kutta methods*, which are of the form

$$\phi(h, u) = u + h \sum_{i=0}^{m} \beta_i k_i(h, u) \tag{5.3}$$

with $k_0(h, u) = f(u)$ and

$$k_i(h, u) = f(u + h \sum_{j=0}^{i-1} \beta_{ij} k_j(h, u)), \ i = 1, \ldots m.$$

As in (1.7), let us assume that the one step mapping $\phi : [0, h_0] \times \mathbb{R}^N \to \mathbb{R}^N$ is smooth and defines a method of order p, i.e., let

$$\phi(h, v) = \Phi(h, v) + \mathcal{O}(h^{p+1}) \tag{5.4}$$

holds uniformly in any bounded v-set. For Runge-Kutta methods this condition is used for determining the coefficients. Due to the smoothness of ϕ and Φ we may restate (5.4) as

$$\frac{\partial^i \phi}{\partial h^j}(0, v) = \frac{\partial^j \Phi}{\partial h^j}(0, v), \ j = 0, \ldots p, \ v \in \mathbb{R}^N. \tag{5.5}$$

Differentiating this relation with respect to v, we find by a Taylor-expansion at $h = 0$ that also

$$\phi_v(h, v) = \Phi_v(h, v) + \mathcal{O}(h^{p+1}) \tag{5.6}$$

holds uniformly in bounded v-sets. Therefore, the sensitivity of the discrete flow to perturbations of the initial value is close to the sensitivity of the continuous flow with the same order of accuracy. This argument can be continued for higher derivatives, but of course the constants in front of h^{p+1} may grow in general. Since discrete and continuous h-flows are so close, one might think, that it is possible to interpret a discrete h-flow as the continuous h-flow of a perturbed dynamical system. More explicitly,

given the system (5.1) and the one-step method (5.2), do there exist smooth functions

$$F_h : \mathbb{R}^N \to \mathbb{R}^N$$

such that for sufficiently small h

$$\phi(h, u, f) = \Phi(h, u, F_h), \quad u \in \mathbb{R}^N? \tag{5.7}$$

This would allow us to use the perturbation results on dynamical systems, in particular those on structural stability, for analyzing one-step methods. However, (5.7) is false in general. For example, take $N = 1$, $f(u) = u^2$ and Euler's method. Then $\phi(h, u, f) = u + hu^2$ is not a diffeomorphism, but $\Phi(h, \cdot, F_h)$ is a diffeomorphism, whatever F_h looks like. This example relies on the global behaviour of the discrete flow, but it is also very likely that (5.7) does not hold locally, i.e. for some u-neighbourhood. But we don't know of any rigorous proof.

In contrast to the negative statements above, there is an elementary class of functions f, where (5.7) does hold. This is the linear case $f(u) = Au$, $A \in \mathbb{R}^{N,N}$. For all common methods, e.g. the Runge Kutta methods, the discrete h-flow is of the form

$$\phi(h, u, A) = g(hA)u$$

where $g(z)$ is a complex function, which is holomorphic in a neighbourhood of zero. g is usually called the *growth function* of the one-step method. If the method is of order p, then we obtain from (5.6) the well-known relation

$$g(hA) = e^{hA} + \mathcal{O}(|h|^{p+1}). \tag{5.8}$$

Now we use the logarithm, holomorphic near 1, in order to define

$$A_h = \frac{1}{h} \ln[g(hA)], \quad h > 0, \quad A_0 = A.$$

From (5.8) we find

$$A_h = \frac{1}{h} (hA + \mathcal{O}(h^{p+1})) = A + \mathcal{O}(h^p)$$

and the relation (5.7)

$$\Phi(h, u, A_h) = e^{hA_h}u = g(hA)u = \phi(h, u, A).$$

In other words, one-step methods applied to linear systems, yield h-flows of a perturbed linear system which is close to the original one within the order of the method.

5.5.2   Persistence of compact invariant sets under discretization

In general we would like to know, if for any compact invariant set M of the flow Φ we can find a compact set $M_h \subset \mathbb{R}^N$ which is *invariant under* $\phi(h, \cdot)$ (i.e. $v \in M_h \Rightarrow \phi(h, v) \in M_h$ and $\phi(h, w) \in M_h \Rightarrow w \epsilon M_h$) and which satisfies

$$H(M, M_h) \to 0 \quad \text{as} \quad h \to 0. \tag{5.9}$$

Here $H(M_1, M_2)$ is the *Hausdorff distance* of two closed sets $M_1, M_2 \subset \mathbb{R}^N$ given by

$$
\begin{aligned}
H(M_1, M_2) &= \text{Max}(\text{dist}(M_1, M_2), \ \text{dist}(M_2, M_1)) \\
\text{dist}(M_1, M_2) &= \sup_{u \in M_1} \inf_{v \in M_2} \|u - v\|.
\end{aligned}
$$

In addition, we would like M_h to inherit the stability properties of M. For stationary points such an asymptotic result is easily established (see Theorem 5.1 below). This contrasts with the variety of spurious solutions that may arise with growing h (cf. the references cited in 5.1.2). In spite of these spurious effects, let us notice that most one-step methods have all stationary points of $\dot{u} = f(u)$ as exact fixed points for all $h > 0$. For example, this is easily verified for the Runge-Kutta methods (5.3). Nevertheless, the following global result is instructive.

Theorem 5.1. *Let $\Omega \subset \mathbb{R}^N$ be compact and assume that (5.1) has finitely many stationary points v_i, $i = 1, \ldots K$ in the interior of Ω (which are unique in Ω) and assume these to be regular, i.e.,*

$$f'(v_i) \text{ is invertible for } i = 1, \ldots K.$$

Let ϕ be a smooth one-step method of order $p \geq 1$. Then there exists an $h_0 > 0$, such that the discrete h-flow $\phi(h, \cdot)$, $h \leq h_0$, has exactly K fixed points $v_i(h)$, $i = 1, \ldots K$ in Ω and these satisfy

$$v_i(h) = v_i + \mathcal{O}(h^p), \quad i = 1, \ldots, K. \tag{5.10}$$

Moreover, if Re $\mu > 0$ for some eigenvalue μ of $f'(v_i)$ then $v_i(h)$ is an unstable fixed point for $\phi(h, \cdot)$, and if Re $\mu < 0$ for all eigenvalues μ of $f'(v_i)$ then it is an asymptotically stable fixed point.

Proof. For the construction of the fixed points let us define the smooth function

$$g(h, v) = \frac{1}{h} \left(\phi(h, v) - v \right) = \int_0^1 \frac{\partial \phi}{\partial h} (sh, v) \, ds. \tag{5.11}$$

Using (5.5) we obtain

$$g(0,v) = \frac{\partial \phi}{\partial h}(0,v) = \frac{\partial \Phi}{\partial h}(0,v) = f(v) \qquad (5.12)$$

and $g_v(0,v) = f'(v)$. Therefore we can apply the implicit function theorem to the equation $g(h,v) = 0$, with (h,v) in a neighbourhood of $(0,v_i)$. This gives us the existence and local uniqueness of the fixed points $v_i(h)$. Moreover, (5.10) follows from

$$g(h,v_i) = \frac{1}{h}(\Phi(h,v_i) + \mathcal{O}(h^{p+1}) - v_i) = \mathcal{O}(h^p).$$

Now we take any sequence v_h of fixed points for $\phi(h,\cdot)$ in Ω where $h \to 0$. Then we can assume $v_h \to \bar{v} \in \Omega$ for some subsequence $h \to 0$ and find from (5.12)

$$0 = g(h,v_h) \to g(0,\bar{v}) = f(\bar{v}) \quad \text{as } h \to 0.$$

Thus $\bar{v} = v_i$ for some i, and v_h must enter the uniqueness neighbourhood for $v_i(h)$ and hence coincide with $v_i(h)$. This establishes the global uniqueness of the fixed points $v_i(h)$ in Ω. Finally, by differentiating (5.11) we obtain

$$A_h := g_v(h,v_i(h)) = \frac{1}{h}(\phi_v(h,v_i(h)) - I) \to g_v(0,v_i) = f'(v_i)$$

as $h \to 0$. Therefore,

$$\phi_v(h,v_i(h) = I + hA_h$$

has an eigenvalue of modulus larger than 1, if $f'(v_i)$ has an eigenvalue with positive real part. Similarly, all eigenvalues of $\phi_v(h,v_i(h))$ lie inside the unit circle if those of $f'(v_i)$ are in the negative half plane. The standard analogoue of Theorem 1.1 for the stability of fixed points (see Irwin[51]) then yields the desired result. ∎

A corresponding result for periodic orbits is considerably more involved. It was shown by Braun and Hershenov[16] that a one-step method has an invariant circle for sufficiently small h close to an asymptotically stable periodic orbit. This was generalized by Doan[26] to the hyperbolic case and further details, in particular on the estimates, were developed by Beyn[8], Eirola[32,33]. The general result is

Theorem 5.2. *Assume that $\dot{u} = f(u)$ has a hyperbolic periodic orbit (cf. 2.2, 2.3, 2.4)*

$$\gamma = \{\bar{u}(t) : 0 \le t \le T\}$$

and let ϕ be a smooth one-step method of order p. Then for h sufficiently small there exists an invariant curve γ_h for the discrete h-flow which is $\mathcal{O}(h^p)$ close to γ. More precisely, we have

$$\gamma_h = \{\overline{u}_h(t) : 0 \leq t \leq T\},$$

where $\overline{u}_h : \mathbb{R} \to \mathbb{R}^N$ is a T-periodic Lipschitz function, and

$$\|\overline{u}(t) - \overline{u}_h(t)\| \leq C \, h^p \text{ for } 0 \leq t \leq T \tag{5.13}$$

$$\phi(h, \overline{u}_h(t)) = \overline{u}_h(\widetilde{\phi}(t, h)), \;\; \widetilde{\phi}(t, h) = t + h + \mathcal{O}(h^{p+1}) (t \in \mathbb{R}). \tag{5.14}$$

Clearly, (5.13) gives us the desired result $H(\gamma, \gamma_h) = \mathcal{O}(h^p)$, but some more information is contained in (5.14). The mapping $t \to \widetilde{\phi}(t, h)$ may be regarded as the reduced discrete h-flow on the invariant curve and its *rotation number* is found to be $\frac{h}{T} + \mathcal{O}(h^{p+1})$ (see Beyn[8]). It is also true that, if the stability or instability criteria from Theorem 2.2 are satisfied for γ, then also γ_h is asymptotically stable respectively unstable. Consider a system with an asymptotically stable periodic orbit and apply a one-step method. If we plot the points of the iteration on a screen then we usually see the invariant curve gradually filled up by pixels (cf. Brezzi, Fujii and Ushiki[17], Beyn[8] for some illustrations). The reason for the fill up is that the rotation number of $\widetilde{\phi}$, obtained by a random choice of h, is 'sufficiently irrational'. For larger values of h, however, periodic orbits with a finite number of points are quite typical.

Let us mention that Eirola[33] used in his proof a general theorem of Hirsch, Pugh and Shub[47] on the persistence of so-called *normally hyperbolic invariant manifolds*. This suggests that Theorem 5.2 may be generalized to this type of invariant manifolds. But no detailed investigations seem to be available up to now.

For the specific case of center manifolds, however, there is a corresponding result by Beyn and Lorenz[14]. Let $v \in \mathbb{R}^N$ be a stationary but nonhyperbolic point of (5.1). Then the linearization $f'(v)$ induces a splitting $\mathbb{R}^N = X \oplus Y$ where X (respectively Y) are invariant subspaces spanned by the (generalized) eigenvectors which belong to the eigenvalues on (respectively off) the imaginary axis. Under these assumptions there exists a center manifold, i.e. a locally invariant manifold of the form

$$M = \{u = (x, y(x)) : x \in X, \; \|x - v\| < \epsilon\}$$

with $y'(v) = 0$. Under some technical assumptions, it is then shown that any p-th order one-step method also has a locally invariant manifold of the form

$$M_h = \{u = (x, y_h(x)) : x \in X, \; \|x - v\| < \epsilon\},$$

such that $y_h(x) = y(x) + \mathcal{O}(h^p)$. This again gives us $H(M, M_h) = \mathcal{O}(h^p)$. The result should be carefully interpreted, however, for the following two reasons. First, the center manifold M is usually not unique, though all center manifolds are tangent to each other to all orders. The manifolds M and M_h are therefore selected out of a possible continuum of manifolds. Second, M_h is not necessarily a center manifold for $\phi(h, \cdot)$, because eigenvalues μ of $f'(v)$ with $Re\,\mu = 0$ might lead to stable or unstable eigenvalues of the linearization $\phi_v(h, v)$ (see the proof of Theorem 5.1).

In view of our treatment of direct methods in chapters 2 to 4, it is natural to continue the previous discussion for parametrized systems

$$\dot{u} = f(u, \lambda), \ u(t) \in \mathbb{R}^N, \ \lambda \in \mathbb{R}. \tag{5.15}$$

There are still many open questions in this field and so we just briefly mention a few results and problems. As mentioned above, stationary points are usually reproduced exactly as fixed points for common one-step methods. This also applies to the stationary bifurcation diagram of (5.15), so that there are no problems.

The next step is the analysis of one-step methods

$$u^{n+1} = \phi(h, u^n, \lambda) \tag{5.16}$$

in the neighbourhood of some λ_0, where the system (5.15) undergoes a Hopf bifurcation (cf. 5.3.4). For this case a corresponding result is given (with a sketch of proof) for Euler's method in Brezzi, Fujii and Ushiki[17]. According to their result, a branch of invariant circles for the map $\phi(h, \cdot)$ bifurcates off at some $\lambda_h = \lambda_0 + \mathcal{O}(h)$.

Let us write down for an illustration Euler's method for the example $1(-\lambda)$ in 5.3.4

$$\phi(h, u) = (x + hy, y + h(\lambda - 2y - x^2 + xy)), \ u = (x, y).$$

At the stationary points $(\sqrt{\lambda}, 0)$ we find

$$\phi_u(h, \sqrt{\lambda}, 0) = \begin{pmatrix} 1 & h \\ -2h\sqrt{\lambda} & 1 + h(\sqrt{\lambda - 2}) \end{pmatrix}.$$

A short calculation reveals that this matrix has two complex conjugate eigenvalues for λ close to 4, and these two eigenvalues cross the unit circle at

$$\lambda_h = \left(\frac{2}{1 + 2h}\right)^2 = 4 + \mathcal{O}(h).$$

At this point the invariant curves are born according to the theorem of *Hopf bifurcation for maps* (see e.g., Iooss[50]) and this is the technique used by Brezzi, Fujii and Ushiki[17].

An attempt to understand (5.16) in the neighbourhood of a homoclinic bifurcation was made in Beyn[9]. From some numerical experiments it was conjectured that the homoclinic structure is preserved by the one-step mapping in the case of a smooth system (5.15) but destroyed otherwise. This conjecture seems to be false, but the case is still under investigation and details will appear elsewhere. For the remaining two bifurcations with periodic orbits, i.e. the period doubling and the torus bifurcation, we don't know of any results concerning the behaviour of the one-step mapping.

Let us conclude this section with a reference to the paper of Kloeden and Lorenz[61]. It is the only one which deals with a general attracting set of the dynamical system. They assume that the given system (5.1) has a compact invariant set $M \subset \mathbb{R}^N$ which is *uniformly asymptotically stable*, i.e., there exists a $\delta > 0$ and for each $\epsilon > 0$ a time $T(\epsilon)$ such that that

$$\text{dist}(\Phi(t, u^0), M) \leq \epsilon \text{ if } t \geq T(\epsilon) \text{ and } \text{dist}(u^0, M) \leq \delta.$$

Under this assumption they show that a one-step method of order p has a compact positively invariant set of the form

$$M_h = \{u \in \mathbb{R}^N : u \in U, \ V(u) \leq C \ h^p\}. \tag{5.17}$$

Here U is some suitable open neighbourhood of M and

$$V : U \to \mathbb{R}$$

is a Lipschitz continuous Liapunov function which decreases along trajectories, is identically zero on M and satisfies an estimate

$$\alpha(\text{dist}(u, M)) \leq V(u) \leq \beta(\text{dist}(u, M)) \tag{5.18}$$

where $\alpha, \beta : \mathbb{R}_+ \to \mathbb{R}_+$ are continuous, strictly increasing functions. The existence of such a Liapunov function follows from the stability assumption by a general theorem of Yoshizawa[101]. From (5.17) one obtains the convergence in the Hausdorff distance, more precisely

$$H(M, M_h) = \mathcal{O}(\alpha^{-1}(h^p)).$$

Of course, in general V, α, β are not known explicitly. Also the positively invariant sets are rather 'thick', because they consist of shrinking neighbourhoods of the continuous attractor. In fact, they absorb the discrete trajectories in a uniform time. Nevertheless, this kind of result seems to be the only one possible under such general assumptions.

5.5.3 Comparison of trajectories

Let us finally return to the problem of estimating the global discretization error on the positive real axis (compare (1.8)). If the system $\dot{u} = f(u)$ has some kind of sensitive dependence on initial conditions, then it is conceivable that also discrete and continuous trajectories will go apart after some time even if the step-size h is small and if the continuous trajectory stays bounded for all times (see also Fig. 5.20 below). The simplest situation of this type occurs in the neighbourhood of a hyperbolic unstable stationary point. There the longtime behaviour of a trajectory depends on the position of the initial value above, below or on the stable manifold. Let us consider for illustration the scalar example

$$\dot{u} = \lambda u, \quad u(0) = u^0, \tag{5.19}$$

where $\lambda \in C$ and $u(t) \in C^N$, and take the familiar one-step method ($\Theta \in [0,1]$)

$$\frac{u^{n+1} - u^n}{h} = \Theta(\lambda u^{n+1}) + (1 - \Theta)(\lambda u^n), \quad n = 0, 1, 2, \ldots. \tag{5.20}$$

For the solutions

$$\Phi(t, u^0) = e^{\lambda t} u^0, \tag{5.21}$$

$$\Psi(nh, u^0) := u^n = [g(h\lambda)]^n u^0, \quad g(z) = \frac{1 + (1 - \Theta)z}{1 - \Theta z}$$

one readily verifies in the case $Re\ \lambda < 0$, $|u^0| \leq 1$

$$|\Phi(nh, u^0) - \Psi(nh, u^0)| \leq C_\lambda h^p \quad \text{for } n \geq 0 \text{ and } 0 < h \leq h_0. \tag{5.22}$$

Here C_λ is a constant independent of Θ and h, and $p = 2$ if $\Theta = \frac{1}{2}$ and $p = 1$ otherwise.

In the unstable case $Re\ \lambda > 0$ an estimate of type (5.22) is impossible, even if we restrict n, h such that $\Phi(nh, u^0)$ is bounded, say $|\Phi(nh, u^0)| \leq 1$. Take, for example, $\lambda \in \mathbb{R}$, $\lambda > 0$ and Euler's method. Let n be the integer part of $1 + 1/(h\lambda)^2$ and consider the initial value $u^0 = \exp(-nh)$. Then, by construction $\Phi(nh, u^0) = 1$, but

$$\Psi(nh, u^0) = \exp(n(\ln(1 + h\lambda) - h\lambda))$$

$$= \exp(n(-\frac{1}{2}(h\lambda)^2 + \mathcal{O}(h\lambda)^3))$$

$$\leq \exp(-\frac{1}{2} + \mathcal{O}(h\lambda)).$$

Therefore $\Phi(nh, u^0) - \Psi(nh, u^0)$ is of order 1, no matter how small h is chosen. However, it is possible in the unstable case $Re\ \lambda > 0$ to find a suitable initial value $v^0 \in \mathbb{R}$ such that

$$|\Phi(nh, u^0) - \Psi(nh, v^0)| \leq C_\lambda h^p \qquad (5.23)$$

holds for $|u^0| \leq 1$ and for all n, h with $|\Phi(nh, u^0)| \leq 1$. In the case $u^0 = 0$ we can take $v^0 = 0$, but in the case $0 < |u^0| \leq 1$ we construct v^0 as follows. The solution of (5.19) reaches the unit circle at time $T = -(\ln|u^0|)/(Re\lambda)$; let n_0 be the integer part of T/h and define

$$v^0 = u^0 \left(\frac{\exp(h\lambda)}{g(h\lambda)}\right)^{n_0}. \qquad (5.24)$$

Then we have identical final values $\Phi(n_0 h, u^0)$ and $\Psi(n_0 h, v^0)$ within the unit circle, and (5.23) follows from (5.22) since the Θ-method for (5.19) is the reverse of the $(1 - \Theta)$-method for $\dot{u} = -\lambda u$.

We notice that the scaled initial value v^0 depends on h, λ and u^0, but not on n in (5.23). This elementary result easily carries over to general linear systems

$$\dot{u} = Au,$$

where $A \in \mathbb{R}^{N,N}$ is hyperbolic and diagonalizable. We transform into a diagonal system, then adjust the initial values for unstable eigenvalues as in (5.24) and transform back to the original variables.

It was shown in Beyn[10] that estimates of the form (5.23) also hold in the neighbourhood of hyperbolic stationary points.

Theorem 5.3. *Let 0 be a hyperbolic stationary point of (5.1) and let it be a fixed point of the one-step mapping $\phi(h, \cdot)$ for all h. Moreover, let ϕ be smooth and consistent of order p (cf. (5.4)). Then there exist constants c, ϵ, h_0 such that for any $u^0 \in \mathbb{R}^N$, $||u^0|| \leq \epsilon$ and $0 < h \leq h_0$ there exists a $v^0 = v^0(u^0, h) \in \mathbb{R}^N$ with the property*

$$||\Phi(nh, u^0) - \Psi(nh, v^0)|| \leq Ch^p \qquad (5.25)$$

for all n such that $||\Phi(t, u^0)|| \leq \epsilon$ for $t \in [0, nh]$. Here $\Psi(nh, v^0)$ denotes the solution of (5.2) with initial value v^0. Conversely, for any $v^0 \in \mathbb{R}^N$, $||v^0|| \leq \epsilon$ and $h \leq h_0$ there exists a $u^0 = u^0(v^0, h)$ such that (5.25) holds for all n with $||\Psi(jh, v^0)|| \leq \epsilon$, $(j = 0, \ldots, n)$.

Loosely speaking this theorem shows that any discrete trajectory approximates *some* continuous trajectory (and vice versa), as long as it stays in some neighbourhood of the hyperbolic point. Thus in this case, the adjustment of initial values saves the uniform estimate. One should notice
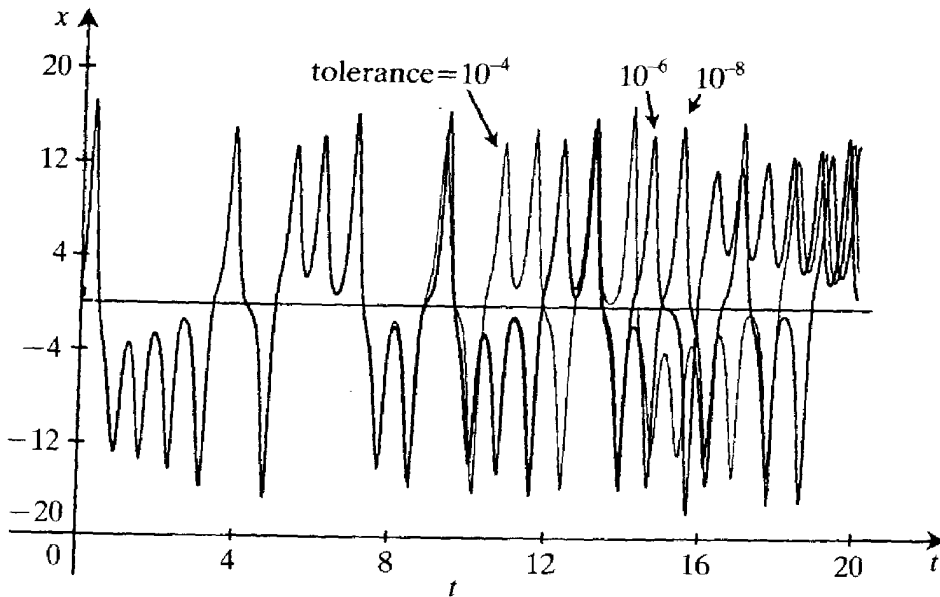
Fig. 5.20. Time diagram for the numerical approximation of trajectories in the Lorenz system $(\sigma = 10,\ \mu = 8/3,\ \lambda = 28)$, initial value $u^0 = (1, 4, 9)$

that the set of n-values for which (5.25) holds can be arbitrarily large depending on u^0. In the extreme case when u^0 is on the stable manifold of the stationary point, then (5.25) holds for all $n \geq 0$. In fact, the fixed point of the one-step mapping $\phi(h, \cdot)$ has a stable manifold which approximates the continuous one within the order of the method (cf. Beyn[10] and also the various results on invariant manifolds in 5.5.2).

In the neighbourhood of periodic orbits, estimates of the form (5.25) are no longer possible, since the continuous and discrete trajectories inevitably run out of phase after some time (this is documented in Beyn[8]). If the periodic orbit is asymptotically stable, then all we can expect is convergence of the positive trajectories in the Hausdorff metric, (see Beyn[8]), i.e.,

$$H(\gamma_+(u^0),\ \gamma_{+h}(u^0)) \to 0 \quad \text{as } h \to 0,$$

where $\gamma_+(u^0) = \{\Phi(t, u^0) : t \geq 0\}$, $\gamma_{+h}(u^0) = \{\Psi(nh, u^0) : n \geq 0\}$.

For systems with strange attractors or chaotic behaviour such as the Lorenz system (Sparrow[90] or 5.3.6, Example 5) it seems no longer appropriate to try to approximate trajectories over large time intervals. This is clearly demonstrated in Figure 5.20 which shows three numerical time diagrams for the Lorenz equations $(\sigma = 10, \mu = \frac{8}{3}, \lambda = 28)$ obtained with a standard ordinary differential equation-solver and three different

tolerances. All of them go apart, and it can be estimated that even if the tolerance is taken to be the machine precision ($\sim 10^{-16}$) then accurate trajectories can be expected at most up to $t = 50$. As a consequence of this well-known effect one should rather compare certain quantities measured from the numerical trajectories with their continuous counterparts, such as Liapunov exponents. Although methods for calculating Liapunov exponents numerically have become quite popular (see e.g. Shimada and Nagashima[89], Kubiček and Marek[63], Seydel[87]), there seems to be no rigorous justification of these methods however simple the system may be. This does not come as a surprise since the proof of existence for these exponents is already a considerable task (see Oseledec[75]).

References

[1] E. L. Allgower and K. Georg, *Numerical continuation methods, an introduction*, Springer Series in Computational Mathematics, 13, Springer, New York, 1990.

[2] J. P. Abbott, *An efficient algorithm for the determination of certain bifurcation points*, J. Comput. Appl. Math. 4, 1978, 19-27.

[3] H. Amann *Gewöhnliche Differentialgleichungen*, De Gruyter, Berlin, 1983.

[4] A.A. Andronov, E. A. Leontovich, I.I. Gordon and A. G. Maier, *Theory of bifurcations of dynamical systems on a plane*, Wiley, New York, 1973.

[5] V. I. Arnold *Ordinary differential equations*, MIT Press, Cambridge, 1973.

[6] U. M. Ascher, R. M. M. Mattheij and R. D. Russell *Numerical solution of boundary value problems for ordinary differential equations*, Prentice Hall, 1988.

[7] W.-J. Beyn *Defining equations for singular solutions and numerical applications*, 42-56 in Küpper, Mittelmann, Weber (Eds. 1984).

[8] W.-J. Beyn *On invariant closed curves for one-step methods*, Numer. Math. 51, 1987, 103-122.

[9] W.-J. Beyn *The effect of discretization on homoclinic orbits*, 1-8 in Küpper, Seydel, Troger (Eds. 1987).

[10] W.-J. Beyn *On the numerical approximation of phase portraits near stationary points*, SIAM J. Numer. Anal. 24, 1987, 1095-1113.

[11] W.-J. Beyn *The numerical computation of connecting orbits in dynamical systems*, IMA J. Numer. Anal., 1990, 379-405.

[12] W.-J. Beyn *Global bifurcations and their numerical computation*, In B. De Dier, D. Roose and A. Spence (Eds. 1990).

[13] W.-J. Beyn *Global bifurcations near singular points*, In preparation, 1990.

[14] W.-J. Beyn, Lorenz, J. *Center manifolds of dynamical systems under discretization* , Numer. Funct. Anal. Optimiz. 9, 1987, 381-414.

[15] R.I. Bogdanov, *Versal deformations of a singular point on the plane in the case zero eigenvalues*, Functional Anal. and its Appl. 9, 1975, 144-145.

[16] M. Braun and J. Hershenov, *Periodic solutions of finite difference equations*, Quart. Appl. Math. 35, 1977, 139-147.

[17] F. Brezzi, H. Fujii and S. Ushiki, *Real and ghost bifurcation dynamics in difference schemes for ODEs*, 79-104 in Küpper, Mittelmann, Weber (Eds. 1984), 1984.

[18] J. Carr, *Applications of center manifold theory*, Springer, New York, 1981.

[19] T. F. Chan, *Deflation techniques and block-elimination algorithms for solving bordered singular systems*, SIAM J. Sci. Stat. Comput. 5, 1984, 121-134.

[20] S.-N. Chow and J. K. Hale, *Methods of bifurcation theory*, Grundlehren der math. Wiss. 251, Springer, New York , 1982.

[21] W. A. Coppel, *Dichotomies in stability theory*, Lecture Notes in Mathematics 629, Springer, 1978.

[22] F. R. De Hoog and R. Weiss, *An approximation theory for boundary value problems on infinite intervals*, Computing 24, 1980, 227-239.

[23] B. De Dier, D. Roose and P. Van Rompay, *Interaction between fold and Hopf curves lead to new bifurcation phenomena*, J. of Comp. Appl. Math. 26, 1989, 171-186.

[24] B. De Dier, D. Roose and A. Spence, (eds.), *Continuation and bifurcations: Numerical technique and applications*, to appear in NATO ASI Series Kluwer, Dordrecht, 1990.

[25] L. Dieci, J. Lorenz and R. D. Russell, *Numerical calculation of invariant tori*, to appear in SIAM J. Sci. Stat. Comput., 1990.

[26] H. T. Doan, *Invariant curves for numerical methods*, Quart. Appl. Math. 43, 1985, 385-393.

[27] E. J. Doedel, *AUTO: A program for the automatic bifurcation analysis of autonomous systems*, Congressus Numerantium 33, 1981, 115-146.

[28] E. J. Doedel and J. P. Kernévez, *AUTO: Software for continuation and bifurcation problems in ordinary differential equations*, Appl. Math. Technical Report, Caltech, 1986.

[29] E. J. Doedel and M. J. Friedman, *Numerical computation of heteroclinic orbits*, J. of Comp. Appl. Math. 26, 1989, 155-170.

[30] E. J. Doedel and M. J. Friedman, *Numerical computation and continuation of invariant manifolds connecting fixed points with application to computation of combustion fronts*, To appear in Proc. of 7th Int. Conf. on FEMIF, 1990.

[31] E. J. Doedel and M. J. Friedman, *Numerical computation and continuation of invariant manifolds connecting fixed points*, Preprint, University of Alabama, Huntsville, 1990.

[32] T. Eirola, *Invariant circles of one-step methods*, BIT 28, 1988, 113-122.

[33] T. Eirola, *Two concepts for numerical periodic solutions of ODE's*, Appl. Math. Comput. 31, 1989, 121-131.

[34] B. Fiedler, *Global Hopf bifurcation of two-parameter flows*, Arch. Rat. Mech. Anal. 94, 1986, 59-81.

[35] C. Foias, M. S. Jolly, I. G. Kevrekidis, G. R. Sell and E.S. Titi, *On the computation of inertial manifolds*, Physics Letters A 131, 1988' 433-436.

[36] E. Freire, E. Ponce and A. J. Rodriguez-Luis, *Un método de continuación de órbitas homoclinas en sistemas autonomos planos biparametricos* , Preprint, Universidad de Sevilla, 1989.

[37] T. Garrett, G. Moore and A. Spence *The detection of Hopf bifurcation points* , In B. De Dier, D. Roose and A. Spence, Ed. 1990.

[38] P. Glendinning, *Global bifurcations in flows*, In New Direction in *Dynamical Systems* (T. Bedford, J. Swift (Eds.)), London Math. Soc. Lecture Notes Series 127, Cambridge University Press, 1988, 120-149.

[39] W. Govaerts, *Stable solvers and block-elimination for bordered systems*, to appear in SIAM J. Matrix Analysis Appl.

[40] A. Griewank and G. W. Reddien, *The calculation of Hopf points by a direct method*, IMA J. Numer. Anal. 3, 1983, 295-303.

[41] A. Griewank and G. W. Reddien, *Characterization and computation of generalized turning points*, SIAM J. Numer. Anal. 21, 1984, 176-185.

[42] A. Griewank and G. W. Reddien, *Computation of cusp singularities for operator equations and their discretizations*, J. of Comp. Appl. Math. 26, 1989, 133-153.

[43] J. Guckenheimer and Ph. Holmes, *Nonlinear oscillations, dynamical systems, and bifurcations of vector fields*, Appl. Math. Sci. 42, Springer, New York, 1983.

[44] J. Hale, *Ordinary differential equations*, Wiley, New York , 1969.

[45] J. Hale, *Introduction to dynamic bifurcation*, in *Bifurcation Theory and Applications* (L. Salvadori, Ed.), Springer, Lecture Notes in Mathematics 1057, 1983.

[46] B. D. Hassard, N. D. Kazarinoff, and Y.-H. Wan, *Theory and applications of Hopf bifurcation* , London Math. Soc. Lecture Note Series 41, 1981.

[47] M. W. Hirsch, C. Pugh, and M. Shub, *Invariant manifolds*, Springer, Lecture Notes in Mathematics 583, 1977.

[48] M. W. Hirsch and S. Smale, *Differential equations, dynamical systems, and linear algebra*, Academic Press, New York, 1974.

[49] M. Holodniok, P. Knedlik, and M. Kubiček, M. *Continuation of periodic solutions in parabolic partial differential equations*, in Küpper, Seydel, Troger (Eds. 1987), 1987, 122-130.

[50] G. Iooss, *Bifurcation of maps and applications*, North-Holland, 1979.

[51] M. C. Irwin, *Smooth dynamical systems*, Academic Pres, New York, 1980.

[52] E. Isaacson and H. B. Keller, *Analysis of numerical methods*, Wiley, New York, 1966.

[53] A. Iserles, A. T. Peplow and A. M. Stuart, *A unified approach to spurious solutions introduced by time discretisation, Part I: Basic theory*, Numerical Analysis Report NA 4, DAMTP Cambridge, 1990.

[54] A. D. Jepson, *Numerical Hopf bifurcation*, Thesis, Caltech, Pasadena, 1981.

[55] A. D. Jepson and A. Spence, *Singular points and their computation*, in Küpper, Mittemann, Weber (Eds. 1984), 1984, 195-209.

[56] H. B. Keller, *Practical procedures in path following near limit points*, in *Computing Methods in Applied Sciences and Engineering* (R. Glowinski and J.L. Lions, Eds.), North Holland, 1982.

[57] H. B. Keller and A. D. Jepson, *Steady state and periodic solution paths: their bifurcations and computations*, in Küpper, Mittelmann and Weber, (eds. 1984).

[58] A. I. Khibnik, V. I. Bykov and G. S. Yablonskii, *Parametric portrait of the catalytic oscillator*, Preprint, Institute of Catalysis, USSR Academy of Sciences, Novosibirsk, (in Russian), 1986.

[59] A. I. Khibnik, LINBF: a program for continuation and bifurcation analysis of equilibria up to codimension three In B. De Dier, D. Roose and A. Spence (Eds. 1990).

[60] I. G. Kevrekidis, R. Aris, L. D. Schmidt and S. Pelikan, *Numerical computations of invariant circles of maps*, Physica 16 D, 1985, 243-251.

[61] P. E. Kloeden and J. Lorenz, *Stable attracting sets in dynamical systems and their one-step discretizations*, SIAM J. Numer. Anal. 23, 1986, 986-995.

[62] H.-O. Kreiss and J. Lorenz, *Initial-boundary value problems and the Navier-Stokes equations*, Academic Press, Boston, 1989.

[63] M. Kubiček and M. Marek, *Computational methods in bifurcation theory and dissipative structures*, Springer, New York, 1983.

[64] M. Kubiček and M. Holodniak, *Numerical determination of bifurcation points in steady and periodic solutions – numerical algorithms and examples*, in Küpper, Mittelmann, Weber (Eds. 1984), 1984, 247-270.

[65] T. Küpper, H. D. Mittelmann and H. Weber, (Eds.) *Numerical methods for bifurcation problems*, ISNM 70, Birkhäuser, Stuttgart, 1984.

[66] T. Küpper, R. Seydel and H. Troger, (Eds.) *Bifurcation: Analysis, Algorithms, Applications* , ISNM 79, Birkhäuser, Stuttgart, 1987.

[67] Y. Kuznetsov, *Computation of invariant manifold bifurcations*, In B. De Dier, D. Roose and A. Spence (Eds. 1990).

[68] M. Lentini and H. B. Keller, *Boundary value problems over semi-infinite intervals and their numerical solution*, SIAM J. Numer. Anal. 17, 1980, 577-604.

[69] X.-B. Lin, *Using Melnikov's method to solve Silnikov's problems* Carolina State University, 1989.

[70] J. Lorenz and Van de Velde *Concurrent computations of invariant manifolds*, Preprint, Caltech, Pasadena, 1989.

[71] V. K. Melnikov, *On the stability of the center for time periodic perturbations*, Trans. Moscow Math. Soc. 12, 1963, 1-57.

[72] G. Moore and A. Spence *The calculation of turning points of nonlinear equations*, SIAM J. Numer. Anal. 17, 1980, 567-576.

[73] S. Newhouse, D. Ruelle and F. Takens, *Occurence of strange axiom – A attractors near quasiperiodic flow on T^n, $n \leq 3$*, Comm. Math. Phys. 64, 1978, 35-40.

[74] J. M. Ortega and W. C. Rheinboldt, *Iterative solution of nonlinear equations in several variables*, Academic Press, New York, 1970.

[75] V. I. Oseledec, *A multiplicative ergodic theorem. Lyapunov characteristic numbers for dynamical systems*, Trans. Moscow Math. Soc. 19, 1968, 197-231.

[76] K. J. Palmer, *Exponential dichotomies and transversal homoclinic points*, J. Diff. Equ. 55, 1984, 225-256.

[77] G. Pönisch, *Computing hysteresis points of nonlinear equations depending on two parameters*, Computing 39, 1987, 1-17.

[78] G. Pönisch and H. Schwetlick, *Computing turning points of curves implicitly defined by nonlinear equations depneding on a parameter*, Computing 26, 1981, 107-121.

[79] W. C. Rheinboldt, *Numerical analysis of continuation methods for nonlinear structural problems*, Computing and Structures 13, 1981, 103-113.

[80] W. C. Rheinboldt, *Numerical analysis of parametrized nonlinear equations*, University of Arkansas, Lecture notes in the Math. Sci. 7, Wiley, 1986.

[81] A. J. Rodriguez-Luis, E. Freire and E. Ponce, *A method for homoclinic and heteroclinic continuation in two and three dimensions*, in B. De Dier, D. Roose and A. Spence (Eds. 1990).

[82] D. Roose, *Numerical computation of origins for Hopf bifurcation in a two-parameter problem*, in Küpper. Seydel, Troger (Eds. 1987), 1987, 268-273 .

[83] D. Roose and V. Hlavacek, *A direct method for the comnputation of Hopf bifurcation points*, SIAM J. Appl. Math. 45, 1985, 879-894.

[84] D. Roose and R. Piessens, *Numerical computation of turning points and cusps.*, Numer. Math. 46, 1985, 189-211.

[85] J. M. Sanz-Serna, *Studies in numerical nonlinear stability I. Why do leapfrog schemes go unstable?*, SIAM J. Sci. Stat. Comp. 6, 1985, 923-938.

[86] R. Seydel, *Numerical computation of branch points in nonlinear equations*, Numer. Math. 33, 1979, 339-352.

[87] R. Seydel, *From equilibrium to chaos: practical bifurcation and stability analysis*, Elsevier, New York, 1988.

[88] Shil'nikov *A case of the existence of a denunerable set of periodic motions*, Sov. Math. Dokl. 6, 1965, 163-16.

[89] I. Shimada and T. Nagashima, *A numerical approach to ergodic problems of dissipative type*, Progress of Theoretical Phys. 61, 1979, 1605-1616.

[90] C. Sparrow, *The Lorenz equations: Bifurcations, chaos and strange attractors*, Springer, New York, 1982.

[91] A. Spence and B. Werner, *Non-simple turning points and cusps* , IMA J. Num. Anal. 2, 1982, 413-427.

[92] A. Spence, K. A. Cliffe and A. D. Jepson, *A note on the calculation of paths of Hopf bifurcations*, J. Comp. Appl. Math. 26, 1989, 125-131.

[93] H. J. Stetter, *Analysis of discretization methods for ordinary differential equations*, Springer, Berlin, 1973.

[94] M. Stiefenhofer, *Zur mathematischen Analyse eines biochemischen Schleimpilzmodells*, Diplomarbeit (Universität Konstanz), 1988.

[95] J. Stoer and R. Bulirsch, *Introduction to numerical analysis*, Springer, New York, 1980.

[96] A. M. Stuart, *Nonlinear instability in dissipative finite difference schemes*, SIAM Review 31, 1989, 191-220.

[97] F. Takens, *Singularities of vector fields*, IHES 43, 1974, 47-100.

[98] R. Temam, *Infinite-dimensional dynamical systems in Mechanics and Phyics*, Appl. Math. Sci. 68, Springer, New York, 1988.

[99] M. van Veldhuizen, *A new algorithm for the numerical approximation of an invariant curve* , SIAM J. Sci. Stat. Comput. 8, 1987, 951-962.

[100] S. Wiggins, *Global bifurcations and chaos (analytical methods)* , Appl. Math. Sci. 73, Springer, New York, 1988.

[101] T. Yoshizawa, *Stability theory by Liapunov's second method*, The Mathematical Society of Japan, 1966.

Professor W.-J. Beyn
Falultät für Mathematik
Universität Bielefeld
Postfach 8640
4800 Bielefeld 1
Germany.