## Invariant Manifolds and Global Bifurcations

John Guckenheimer

Department of Mathematics, Cornell University, Ithaca, NY 14853, USA.

Bernd Krauskopf and Hinke M. Osinga Department of Mathematics, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand

Björn Sandstede Division of Applied Mathematics, Brown University, 182 George Street, Providence, RI 02912, USA (Dated: January 2015)

Invariant manifolds are key objects in describing how trajectories partition the phase spaces of a dynamical system. Examples include stable, unstable and center manifolds of equilibria and periodic orbits, quasiperiodic invariant tori and slow manifolds of systems with multiple timescales. Changes in these objects and their intersections with variation of system parameters give rise to global bifurcations. Bifurcation manifolds in the parameter spaces of multi-parameter families of dynamical systems also play a prominent role in dynamical systems theory. Much progress has been made in developing theory and computational methods for invariant manifolds during the past 25 years. This article highlights some of these achievements and remaining open problems.

Computer investigations of dynamical systems have become a indispensable tool throughout the sciences. These studies often focus upon the geometry of the phase space of the system. Based upon the concepts of genericity and transversality, dynamical systems theory describes typical behaviors. These descriptions involve invariant manifolds of dimension larger than one, such as the stable and unstable manifolds of equilibrium points and periodic orbits. Tangency of pairs of invariant manifolds has been shown to be a key ingredient in some types of global bifurcations in a system. This brief survey describes a few examples of this phenomenon. It highlights numerical methods that identify invariant manifolds and locate their intersections. The examples center around aspects of the FitzHugh-Nagumo equation that has become a prototype for studying traveling waves in dynamical systems described by partial differential equations.

## I. INTRODUCTION

Dynamical systems theory embodies a geometric view of solutions to ordinary differential equations of the form

$$\dot{x} = f(x, \eta), \qquad x \in \mathbb{R}^n, \eta \in \mathbb{R}^\ell,$$

where  $\mathbb{R}^n$  is the phase space and  $\mathbb{R}^\ell$  the parameter space. In creating the subject, Poincaré emphasized the planar case n = 2 and generic properties that are typical among the set of all such equations. He described their phase portraits, which show how solution trajectories partition  $\mathbb{R}^2$ . Stable and unstable manifolds of saddles are key entities in the phase portrait of a generic planar system. Each is a pair of trajectories that approach the saddle as  $t \to \pm \infty$ .

Figure 1 displays phase portraits of the *FitzHugh-Nagumo* vector field [1], given by

$$\begin{cases} \dot{v} = w + v - \frac{v^3}{3}, \\ \dot{w} = -\varepsilon \left(av + b + cw\right), \end{cases}$$
(1)

for three different values of the system parameter  $\varepsilon$  and fixed suitable choices of a, b and c. There are three equilibria in Fig. 1(a)–(c): the upper-left equilibrium is a sink, the lower-right equilibrium is a source, and the middle eqilibrium is a saddle, denoted **p**; moreover there is also an outer stable periodic orbit throughout. Panel (b) shows the situation when there is a *homoclinic orbit*  $\Gamma_0$ , which is simultaneously in the stable and unstable manifold of **p**. At this *homoclinic bifurcation*, an unstable periodic orbit  $\Gamma$  emerges from the homoclinic orbit  $\Gamma_0$  as  $\varepsilon$  is decreased. The periodic orbit  $\Gamma$  supplants the stable manifold of  $\mathbf{p}$  as the boundary between the two attractor basins: points near the source are in the basin of attraction of the sink in Fig. 1(a), and they are in the basin of attraction of the outer stable periodic orbit in Fig. 1(c).

This example illustrates the role of invariant manifolds and their intersections in organizing the phase portraits of dynamical systems. The stable and unstable manifolds of a planar saddle are easy to find: each is formed from just two trajectories that can be computed with standard initial value solvers. However, the geometry and the numerical analysis quickly become *much* more complicated when multiple timescales are involved or the dimension of the system increases.

The limit  $\varepsilon = 0$  of the FitzHugh-Nagumo vector field is singular with a whole curve of equilibrium points.



FIG. 1. Phase portraits near a homoclinic bifurcation of the FitzHugh-Nagumo vector field (1) for (a, b, c) = (1.0, 0.05, 1.2); panel (a) for  $\varepsilon = 0.38$  is before, panel (b) for  $\varepsilon = 0.375149$  is approximately at, and panel (c) for  $\varepsilon = 0.37$  is after the homoclinic bifurcation. Shown are equilibria (black dots), the stable manifold (blue curves) of the saddle **p**, the unstable manifold (red curves) of **p**, and periodic orbits (green curves).

With the change of timescale  $t \mapsto t \varepsilon$ , the resulting slow-fast singularly perturbed system is a differentialalgebraic equation (DAE) in the limit  $\varepsilon = 0$ . When b = c = 0, the system reduces to the Van der Pol equation [2] whose relaxation oscillations have inspired much of the development of singular perturbation theory for dynamical systems with multiple timescales. A fundamental aspect of the subject is the presence of invariant *slow manifolds* along which trajectories evolve on the slow timescale. 'Stiff' numerical methods have been developed to compute trajectories along *attract*ing slow manifolds more efficiently than is done with explicit 'non-stiff' methods. However, trajectories may come to places where they leave an attracting slow manifold, and the stiff methods no longer are the ones of choice. Geometric, analytic and numerical methods are all needed in order to develop a full understanding of the dynamics in these circumstances.

Vector fields in dimensions larger than two exhibit a vastly larger range of phenomena than planar vector fields. Beginning in the 1950's with the work of Kolmogorov [3], KAM theory has shown that invariant tori are quite common in both conservative and dissipative dynamical systems. Enormous effort has gone into studying chaotic dynamics since Smale's discoverv in 1960 of the geometric example called the horseshoe [4, 5]. As important as both invariant tori and chaotic dynamics are in dynamical systems theory, neither is discussed here. Our emphasis is upon invariant manifolds that arise as either stable or unstable manifolds of equilibrium points of a vector field or as slow manifolds of a system with multiple timescales. New computational methods have been developed to visualize these objects, and new theory has been developed to explain their role in organizing the dynamics of systems. As in the FitzHugh-Nagumo example, non-transversal

intersections of invariant manifolds can be regarded as *global* bifurcations that separate parameter regions of a system with different qualitative behaviors. The detection of these phenomena has been important in understanding puzzling observations that were difficult to explain in other ways.

Beyond bifurcations, there are circumstances in which non-generic dynamical behavior is important in applications. As an example, we discuss traveling-wave profiles for infinite dimensional dynamical systems defined by partial differential equations (PDEs). The traveling waves are solutions of an equation with the property that they translate spatially in time. These spatial profiles of associated traveling waves are found as homoclinic orbits of a reduction of the PDE to an ordinary differential equation. They arise, for example, in the context of the Hodgkin–Huxley model [6] of action potentials for nerve cells. This model is one of the landmark achievements of 20th century biology, and it motivated significant developments in dynamical systems theory, including the example discussed here. One version of the FitzHugh-Nagumo model is a PDE that has been used to study propagation of such action potentials along nerves.

We have chosen to organize this brief overview of developments in this area by means of three examples that build upon the FitzHugh-Nagumo vector field introduced above. The first example, an inclination-flip bifurcation, illustrates some of the complexity that occurs with homoclinic bifurcations in three-dimensional vector fields. The second example introduces slow-fast systems with two slow and one fast variable. Here, *folded singularities* are a new phenomenon that gives rise to surprising dynamical phenomena such as *mixed-mode oscillations*. Finally, we study the traveling-wave profiles of the FitzHugh-Nagumo PDE. Interspersed with the examples are sections that provide minimal background material for establishing the mathematical setting of our discussion. Following the examples we give a brief overview of some of the numerical methods used in this work.

#### II. BACKGROUND

Manifolds are defined as locally Euclidean topological spaces. The manifolds discussed in this paper are submanifolds of the state spaces and parameter spaces of dynamical systems. Submanifolds of the state space are *invariant* if they are unions of trajectories. We also consider submanifolds with boundary that are *locally invariant*: trajectories enter or leave the submanifold only through its boundary. In topology, submanifolds are often defined *implicitly* as the set of solutions to a system of equations. In contrast, the invariant manifolds of dynamical systems such as stable manifolds are frequently defined by asymptotic properties of trajectories as  $t \to \pm \infty$ . Consequently, theoretical questions concerning the existence and smoothness of invariant manifolds of dynamical systems are subtle, and the development of numerical algorithms for computing them is hardly straightforward. Each type of invariant manifold presents its own set of issues: we give examples that illustrate current research in this area.

Basic theory of manifolds can be viewed as a generalization of linear algebra. The implicit function theorem gives conditions that guarantee that the set of solutions S to a system of m equations q(x) = 0 in  $\mathbb{R}^n$  form a manifold of dimension n-m, namely, the derivative Dgmust have maximal rank m at all points of S. The integer m is the codimension of S and the null space of Dg(x) is the tangent space of S at  $x \in S$ . Two submanifolds  $S_1$  and  $S_2$  are *transverse* if their tangent spaces span  $\mathbb{R}^n$ . Transverse intersections of submanifolds are again submanifolds. Manifolds can also be defined by coordinate charts, atlases and transition functions that glue together coordinate charts on their overlaps. Numerically, continuation methods based upon the implicit function theorem have become a standard tool for computing one-dimensional manifolds. These methods are based on the observation that the curve S defined by a regular system of n-1 equations g(x) = 0 in  $\mathbb{R}^n$ is a trajectory of vector fields that are tangent to the null space of Dg on S. Methods for higher-dimensional manifolds are far less common and their development is an active area of research; see, for example, Ref. [7].

### III. HOMOCLINIC ORBITS IN HIGHER DIMENSIONS

The homoclinic bifurcation of the FitzHugh-Nagumo model (1) shown in Fig. 1 is typical of planar vector fields, where a single periodic orbit bifurcates from the homoclinic orbit and its stability depends on the relative strengths of the two real eigenvalues of the equilibrium involved. At a generic codimension-one homoclinic bifurcation of an equilibrium the dimensions of the stable and unstable manifolds necessarily add up to the dimension of the phase space. Hence, in the plane they are both one-dimensional objects, and they have branches which coincide at the homoclinic bifurcation.

In higher dimensions this is no longer the case: at least one of the two invariant manifolds is of dimension larger than one and, at a homoclinic bifurcation, the stable and unstable manifolds of the equilibrium do not coincide, instead intersecting in a single trajectory – the homoclinic orbit  $\Gamma_0$ . The behaviors associated with homoclinic orbits depend upon the types and magnitudes of the eigenvalues of the equilibrium (through the saddle quantity that determines the stability of nearby periodic orbits), as well as twisting of the flow around the homoclinic orbit. Already in  $\mathbb{R}^3$ , the case we discuss in this paper, the dynamics near a homoclinic orbit may be very complicated and surprising. The overall dynamics is organized by invariant surfaces, in particular, by two-dimensional stable manifolds of equilibria and saddle periodic orbits.

The classical example of Shilnikov [8, 9] considers a saddle focus **p** of a vector field in  $\mathbb{R}^3$  with a homoclinic orbit  $\Gamma_0$ , where one branch of the one-dimensional unstable manifold  $W^{u}(\mathbf{p})$  lies in the two-dimensional stable manifold  $W^{s}(\mathbf{p})$  and, hence, spirals back into  $\mathbf{p}$ . When the saddle quantity is negative so that  $\Gamma_0$  is attracting, then a single stable periodic orbit bifurcates from  $\Gamma_0$ . However, when the saddle quantity is positive and  $\Gamma_0$  is not attracting then there exists a chaotic invariant set of saddle type near  $\Gamma_0$ ; or, equivalently, there are Smale horseshoes in a suitable Poincaré section. This celebrated result by Shilnikov shows that chaotic dynamics can be located by finding a codimension-one homoclinic bifurcation in  $\mathbb{R}^3$ ; here, an important ingredient is the spiraling nature of the flow near the saddle focus **p** due to the existence of complex-conjugate eigenvalues. As a result, the stable manifold  $W^{s}(\mathbf{p})$ , when followed backwards along the homoclinic orbit  $\Gamma_0$ , forms a helix with infinitely many twists as it returns to **p**; see also Ref. [10].

Homoclinic bifurcations in  $\mathbb{R}^3$  to saddle points  $\mathbf{p}$  with two real stable eigenvalues are also typical and can found in many applications. One can ask if and when chaotic dynamics are found near such a homoclinic bifurcation, as in the Shilnikov case. The crucial geometric ingredient to answer this question lies again in how the two-dimensional stable manifold  $W^s(\mathbf{p})$  twists when it returns back to  $\mathbf{p}$  along  $\Gamma_0$ . Under suitable genericity conditions,  $W^s(\mathbf{p})$  accumulates on the onedimensional strong stable manifold  $W^{ss}(\mathbf{p}) \subset W^s(\mathbf{p})$  at the homoclinic bifurcation. Near  $\Gamma_0$  the surface  $W^s(\mathbf{p})$ either forms a cylinder, which is orientable, or a Möbius strip, which is nonorientable. In both cases a single periodic orbit bifurcates from  $\Gamma_0$  that is either orientable (has two positive Floquet multipliers) or nonorientable (has two negative Floquet multipliers); depending on the eigenvalues of **p**, the bifurcating periodic orbit may be attracting, of saddle type or repelling. In short, one does not find chaotic dynamics near a codimension-one homoclinic bifurcation to a real saddle in  $\mathbb{R}^3$ .

However, it turns out that chaotic dynamics can be found near codimension-two homoclinic bifurcations called flip bifurcations, where the stable manifold  $W^{s}(\mathbf{p})$  changes from orientable to nonorientable. This happens when one of the genericity conditions of a codimension-one homoclinic bifurcation is no longer satisfied. The theory of flip bifurcations is reviewed in Ref. [11], where further references can be found. There are two types, called inclination flip and orbit flip bifurcations, and they come in three cases each, denoted **A**, **B** and **C**, as defined by conditions on the eigenvalues of **p**. Importantly, case **C** features the existence of a chaotic saddle. Flip bifurcations have been found in a number of systems, including the Hindmarsh-Rose model of a class of neuronal cells [12], a Van der Pol-Duffing model [13], and in reaction-diffusion systems with nonlocal coupling [14]. Finding a flip bifurcation in a given system not only requires the detection of the homoclinic orbit  $\Gamma_0$ , but also the determination of whether  $W^{s}(\mathbf{p})$  is orientable or not. The capability of detecting flip bifurcations, via the formulation of welldefined test functions (that use the adjoint of the vector field), has been incorporated into the Homcont [15] part of the package AUTO [16]; see also Sec. VI.

#### A. Inclination flip bifurcation of type A

We now show how the stable manifold  $W^s(\mathbf{p})$  at a homoclinic orbit can suddenly change from being a cylinder to being a Möbius strip. To this end we consider an inclination flip of type  $\mathbf{A}$ , which can be found and studied conveniently[17] in the model vector field

$$\begin{cases} \dot{x} = a x + b y - a x^{2} + (\tilde{\mu} - \alpha z) (2 - 3x) x + \delta z, \\ \dot{y} = b x + a y - \frac{3}{2} b x^{2} - \frac{3}{2} a x y - (\tilde{\mu} - \alpha z) 2y - \delta z, \\ \dot{z} = c z + \mu x + \gamma x z + \alpha \beta (x^{2} (1 - x) - y^{2}), \end{cases}$$
(2)

which was constructed and introduced in Ref. [18] to feature different kinds of codimension-two homoclinic bifurcations in an accessible way. The origin  $\mathbf{0}$  is an equilibrium of (2) and, for the choice of parameters

$$a = -0.05, \ b = 1.05, \ c = -1.2, \ \alpha = 0, \beta = 1, \ \gamma = 0, \ \delta = 0, \ \mu = 0, \ \tilde{\mu} = 0,$$
(3)

with  $\alpha = \alpha_{\mathbf{A}} \approx 0.860183$  there is a homoclinic orbit  $\Gamma_0$  to **0** that satisfies all the conditions of a codimensiontwo inclination flip bifurcation **IF** of type **A**. When the parameter  $\alpha$  is varied from  $\alpha = \alpha_{\mathbf{A}}$ , the homoclinic orbit  $\Gamma_0$  persists. However, it changes from an orientable homoclinic orbit for  $\alpha < \alpha_{\mathbf{A}}$ , denoted  $\mathbf{H}_{\mathbf{o}}$ , to a nonorientable (or twisted) homoclinic orbit for  $\alpha > \alpha_{\mathbf{A}}$ , denoted  $\mathbf{H}_{\mathbf{t}}$ .

Figure 2 illustrates how the two-dimensional stable manifold  $W^s(\mathbf{0})$ , when followed along the homoclinic orbit  $\Gamma_0$ , returns to the origin **0**. In this figure the (x, y, z)-space of (2) has been transformed so that the eigenvectors of this saddle are the coordinate axes; hence, the one-dimensional unstable manifold  $W^u(\mathbf{0})$  is tangent at **0** to the vertical axis and the two-dimensional stable manifold  $W^s(\mathbf{0})$  is tangent to the horizontal plane through **0**. On  $W^s(\mathbf{0})$  we also show the strong stable manifold  $W^{ss}(\mathbf{q})$  and a weak trajectory  $\omega_{-}^s$  tangent to the weak stable eigenvector. Note that there is a second equilibrium  $\mathbf{q}$ , which is a saddle focus, and its one-dimensional stable manifold  $W^s(\mathbf{q})$  is also shown in Fig. 2.

The organization of phase space by  $W^{s}(\mathbf{0})$  at the moment of homoclinic bifurcation is presented in Fig. 2(a1), (b) and (c1). To illustrate the orientability of  $W^{s}(\mathbf{0})$ , this surface is divided along the homoclinic orbit  $\Gamma_0$  and  $\omega_{-}^s$  into a solid part and a transparent part. In panels (a1) and (c1), when it is followed (backward in time) along  $\Gamma_0$ , the stable manifold  $W^s(\mathbf{0})$  accumulates on the strong stable manifold  $W^{ss}(\mathbf{0})$ , meaning that it satisfies the genericity conditions of a codimensionone homoclinic bifurcation. In Fig. 2(a1) the solid half returns on the solid side and the transparent half returns on the transparent side. Here  $W^{s}(\mathbf{0})$  forms an orientable surface, namely a cylinder, and we are dealing with an orientable homoclinic bifurcation  $H_o$ . Notice that the cylinder surrounds the secondary equilibrium **q** and its one-dimensional stable manifold  $W^{s}(\mathbf{q})$ . In Fig. 2(c1), on the other hand, the solid half of  $W^{s}(\mathbf{0})$ returns back along  $\Gamma_0$  on the side of the transparent half, and vice versa, so that  $W^{s}(\mathbf{0})$  forms a Möbius strip and we are dealing with a nonorientable homoclinic bifurcation  $\mathbf{H}_{\mathbf{t}}$ . Notice further that, when  $W^{s}(\mathbf{0})$ is nonorientable, it is a much more complicated surface in  $\mathbb{R}^3$ ; in particular,  $W^s(\mathbf{0})$  now accumulates on the curve  $W^{s}(\mathbf{q})$ .

The transition between the two cases  $\mathbf{H}_{\mathbf{o}}$  and  $\mathbf{H}_{\mathbf{t}}$  of codimension one takes place at the codimension-two inclination flip bifurcation **IF** shown in Fig. 2(b). Here, the surface  $W^{s}(\mathbf{0})$  does not close up along  $W^{ss}(\mathbf{0})$ , but instead aligns along the orbit  $\omega_{-}^{s}$ , that is, it returns tangent to the weak stable eigendirection. Hence, the surface  $W^{s}(\mathbf{0})$  is neither orientable nor nonorientable but 'in between' the two cases.

In order to understand the properties of  $W^s(\mathbf{0})$  at  $\mathbf{H}_{\mathbf{o}}$ and  $\mathbf{H}_{\mathbf{t}}$  it is very helpful to consider its intersection set  $\widehat{W}^s(\mathbf{0})$  of  $W^s(\mathbf{0})$  with a sufficiently large sphere that contains  $\Gamma_0$  in its interior. Figure 2(a2) and (c2) show stereographic projections of such a sphere, and panels



FIG. 2. Transition along a curve of homoclinic bifurcation through an inclination flip **IF** of type **A** of (2). Shown are  $W^s(\mathbf{0})$  (blue surface and curves),  $W^u(\mathbf{0})$  (red curve),  $\Gamma_0$  (red curve),  $W^{ss}(\mathbf{q})$  (cyan curve and dots), and the weak trajectory  $\omega_{-}^s$  (light blue curve and dots) at the orientable homoclinic bifurcation  $\mathbf{H}_o$  for  $\alpha = 0.7$  in row (a), at the inclination flip **IF** for  $\alpha = 0.860183$  in (b), and at an nonorientable homoclinic bifurcation  $\mathbf{H}_t$  for  $\alpha = 1.0$  in row (c); the other parameters are as in (3). Panels (a1), (b) and (c1) show the situation in  $\mathbb{R}^3$ ; intersection sets of invariant objects with a sufficiently large sphere are shown in stereographic projection in panels (a2) and (c2), and are sketched in panels (a3) and (c3), at  $\mathbf{H}_o$  and  $\mathbf{H}_t$ , respectively. Images from Ref. [17]. ©2013 Society for Industrial and Applied Mathematics. Reprinted with permission. All rights reserved.

(a3) and (c3) are respective topological sketches. At  $\mathbf{H_o}$  the set  $\widehat{W}^s(\mathbf{0})$  consists of a single curve whose two end points connect up to the curve at the intersection points  $\widehat{W}^{ss}_{-}$  and  $\widehat{W}^{ss}_{+}$  of  $W^{ss}(\mathbf{0})$  with the sphere; see Fig. 2(a2)

and (a3). The resulting two closed curves (one on each side of the sphere) are the intersection set of the cylinder formed by  $W^s(\mathbf{0})$  along  $\Gamma_0$ . What the intersection set of the stable manifold  $W^s(\mathbf{0})$  with the sphere looks

like when  $W^s(\mathbf{0})$  forms a Möbius strip containing  $\Gamma_0$ is less obvious and probably somewhat surprising. As Fig. 2(c2) and (c3) show, at a nonorientable homoclinic bifurcation  $\mathbf{H}_{\mathbf{t}}$  the intersection set  $\widehat{W}^s(\mathbf{0})$  consists of a single closed curve with two arcs that connect the points  $\widehat{W}^{ss}_{-}$  and  $\widehat{W}^{ss}_{+}$  in a spiraling fashion to  $\widehat{W}^s_{-}(\mathbf{q})$ and  $\widehat{W}^{s+}(\mathbf{q})$ , respectively.

The associated two-parameter unfoldings of the codimension-two homoclinic flip bifurcations of type **A** can be found in Ref. [17]. The study of how  $W^s(\mathbf{0})$  organizes the phase space near inclination flip bifurcations of type **B** is ongoing; it involves bifurcating periodic orbits of saddle type and their stable and unstable manifolds, which may be orientable or nonorientable. Finding the structure of invariant manifolds for the most complicated type **C** of inclination flip bifurcations, involving saddle hyperbolic sets with infinitely many saddle periodic orbits, remains an interesting challenge.

#### IV. SLOW-FAST SYSTEMS AND THEIR INVARIANT MANIFOLDS

The FitzHugh–Nagumo vector field (1) is an example of a system with multiple timescales when the parameter  $\varepsilon$  is small. Many aspects of the behavior of such slow-fast systems, particularly in dimensions three and higher, have only recently become better understood through developments in geometric singular perturbation theory [19]. Here, we highlight the analysis of *folded singularities* in systems with two slow and one fast variables as an example of the essential role of invariant manifolds in dynamical systems.

Slow-fast systems are written in their slow timescale as

$$\begin{cases} \varepsilon x' = f(x, y, \eta, \varepsilon), \\ y' = g(x, y, \eta, \varepsilon), \end{cases}$$
(4)

where  $x \in \mathbb{R}^k$  are the fast variables,  $y \in \mathbb{R}^{(n-k)}$  are the slow variables,  $\varepsilon$  is the ratio of timescales and  $\eta \in \mathbb{R}^{\ell}$ are other system parameters. The critical manifold is the set of solutions of the equation  $f(x, y, \eta, 0) = 0$ , and  $y' = g(x, y, \eta, 0)$  defines the slow flow as a differentialalgebraic equation (DAE) when restricted to the critical manifold. Where  $D_x f$  is regular, the implicit function theorem gives  $x = h(y, \eta)$  on the critical manifold and the DAE reduces to an ODE. Furthermore, where  $D_x f$ is hyperbolic, stable manifold theory [20] guarantees the existence of locally invariant slow manifolds close to the critical manifold for small  $\varepsilon > 0$ . Points on the critical manifold where  $D_x f$  is singular are *folds* and the slow flow of the critical manifold is no longer defined. Where folds are simple, the slow flow can be *desingularized* at the expense of changing the direction of time on sheets of the critical manifold where  $det(D_x f) < 0$ . In the full

system with  $\varepsilon > 0$ , trajectories that approach a simple fold 'jump' along the fast direction.

Consider now three-dimensional systems with two slow variables. In these systems, the critical manifold is a two-dimensional surface with attracting and repelling sheets. Trajectories that flow from an attracting sheet to a repelling sheet are *canard orbits* that play a dramatic role in the dynamics. Because repelling slow manifolds are unstable on the fast timescale, the slow-time evolution near these manifolds seems to be discontinuous as trajectories on either side turn away abruptly. Canard orbits appear near *folded singularities*, points on the fold curve where the desingularized system has an equilibrium.

Benoît [21] analyzed the intersections of the attracting and repelling slow manifolds at folded saddles, proving that invariant extensions of the manifolds intersect transversally along canard orbits with an angle that is  $O(\varepsilon)$ . In the singular limit  $\varepsilon = 0$ , the stable manifold of a folded saddle separates trajectories on the attracting slow manifold that flow all the way to the fold curve and then jump, from trajectories that turn away from the fold before reaching it. When  $\varepsilon > 0$ , some trajectories immediately adjacent to the stable manifold form canard orbits that flow onto the repelling slow manifold before jumping. The separation of trajectories along the canard orbits is abrupt and creates the stretching that is characteristic of chaotic invariant sets. Indeed, Haiduc [22] proved that this mechanism explains the landmark results of Littlewood [23–25] on the forced Van der Pol equation [2] that demonstrated the existence of chaotic dynamics in an explicit dissipative system for the first time.

The geometry that is associated with folded nodes is even more complicated and surprising than that of folded saddles. Benoît showed that the attracting and repelling slow manifolds twist as they approach a folded node, creating multiple canard orbits in the process. Benoît [26] and Wechselberger [27] analyzed the amount of twisting that occurs and the bifurcations that produce increasing numbers of canard orbits. The twisting is manifest in small-amplitude oscillations of trajectories that flow past a folded node. When these trajectories have a *global return* to the region around the folded node, they give examples of *mixed-mode oscillations* (MMOs).

#### A. The self-coupled FitzHugh–Nagumo equation

Recently, there has also been increasing interest in MMOs that are observed in the context of neural models. As an example of an MMO that is organized by a folded-node singularity, we consider the FitzHugh– Nagumo equation with synaptic coupling back to itself as a model of single-cell dynamics that is influenced by external electrical signals due to connections to other cells. This model three-dimensional system

$$\begin{cases} \dot{v} = h - \frac{v^3 - v + 1}{2} - \gamma \, s \, v, \\ \dot{h} = -\varepsilon \, (2h + 2.6 \, v), \\ \dot{s} = \beta H(v) \, (1 - s) - \varepsilon \, \delta \, s, \end{cases}$$
(5)

was introduced by Wechselberger [27]. Here, the third variable, denoted s, describes the synaptic coupling, which occurs through voltage v. The parameter  $\gamma$  is the coupling strength. The dynamics of s consists of an activation term, determined by the parameter  $\beta$ , and a deactivation term, controlled by the decay rate  $\delta$ . Activation is only occurring in the active phase, when v > 0, as indicated by the Heaviside function H(v); in the silent phase, when v < 0, the synaptic coupling sdecays on the same timescale as the gating variable h. The presence of the Heaviside function greatly simplifies the analysis of the silent phase, for which system (5) is a slow-fast system with v the fast and h and s the slow variables.

Figure 3(a)-(b) illustrates the response of system (5) for  $\beta = 0.035$ ,  $\gamma = 0.5$ ,  $\delta = 0.565$  and  $\varepsilon = 0.015$ . For these parameters, there exists a stable MMO periodic orbit  $\Gamma_5$  that exhibits five small-amplitude oscillations, which constitute subthreshold oscillations in the silent phase, followed by one large action potential; its v-time series is shown in panel (a). Since H(v) = 0in the subthreshold regime, the structure of slow manifolds for system (5) is independent of  $\beta$  and can be analyzed separately. Slow manifolds of system (5) have also been studied in Ref. [28]. The critical manifold  ${\cal S}$  of system (5) is a cubic surface and a folded node at  $(v, h, s) \approx (-0.4900, 0.6176, 0.2797)$  exists relatively far away from the cusp point at  $(v, h, s) = (0, \frac{1}{2}, 1)$ , on the side of the fold curve with smallest v. Figure 3(b) shows how the intersections between the attracting and repelling slow manifolds of system (5) organize the subthreshold oscillations near the folded node. These slow manifolds were computed with the method explained in Sec. VI. The repelling slow manifold  $S^r_{\varepsilon}$  comprises the family of orbit segments that start in the plane  $\Sigma := \{s = 0.2797\}$  and end on the line  $L^r := \{(v, h, s) \in$  $S \mid v = 0$  = { $(0, \frac{1}{2}, s)$ }. Similarly, the attracting slow manifold  $S^a_{\varepsilon}$  comprises the family of orbit segments that start on the line  $L^a := \{(v, h, s) \in S \mid h = -6\}$  and end in  $\Sigma$ . The slow manifolds  $S_{\varepsilon}^{r}$  and  $S_{\varepsilon}^{a}$  intersect in canard orbits, two of which, namely,  $\xi_4$  and  $\xi_5$ , are highlighted in Fig. 3(b). These canards make four and five smallamplitude oscillations, respectively. As can be seen in Fig. 3(b), the value of  $\beta$  is such that the periodic orbit  $\Gamma_5$  lands (approximately) on  $S^a_{\varepsilon}$  in between the two canard orbits  $\xi_4$  and  $\xi_5$ , which determines the signature of this MMO.

One advantage of our procedure for computing intersections between attracting and repelling slow man-



FIG. 3. (a) Mixed-mode oscillation of system (5) for  $\gamma = 0.5$ ,  $\delta = 0.565$ ,  $\varepsilon = 0.015$  and  $\beta = 0.035$ . (b) Associated attracting and repelling slow manifolds,  $S_{\varepsilon}^{a}$  (red surface) and  $S_{\varepsilon}^{r}$  (blue surface); also shown are the two canard orbits  $\xi_{4}$  (magenta curve) and  $\xi_{5}$  (orange curve); reproduced from Ref. [28]. (c) Continuation in  $\varepsilon$  of the canard orbit  $\xi_{5}$  (while assuming  $H(v) \equiv 0$ ); (d1)–(d4) Projections of  $\xi_{5}$  onto the (s, v)-plane at the correspondingly labeled points along the branch.

ifolds is that we can continue such canard orbits in a system parameter. A particularly interesting parameter is the timescale ratio  $\varepsilon$ ; see also Ref. [29]. Geometric singular perturbation theory predicts the existence and characterization of slow manifolds and canard orbits provided  $\varepsilon$  is small enough. The numerical methods, on the other hand, work for a large range of values of  $\varepsilon$  that extends well beyond the known theory. We have found that these computations yield new predictions about the nature of different canard orbits.

Figure 3(c) illustrates such a numerical exploration with the continuation in  $\varepsilon$  of the canard orbit  $\xi_5$  from panel (b). We plot the  $L_2$ -norm of the continued canard orbit  $\xi_5$ ; the insets (d1)–(d4) show projections onto the (s, v)-plane of four selected canard orbits along the branch. When  $\varepsilon$  is decreased from  $\varepsilon = 0.015$ , we find that  $\xi_5$  accumulates onto the strong canard at  $\varepsilon = 0$ , as predicted by the theory. In the other direction, as  $\varepsilon$  is increased, an interesting transition occurs at  $\varepsilon \approx 0.0305$ , which is close to where the branch has a minimum in the  $L_2$ -norm: the canard orbits change from having s > 0 decreasing, as shown in Fig. 3(b), to having s < 0 increasing; the canard orbits past this transition, including those shown in Fig. 3(d1)-(d4), all satisfy s < 0. We disregarded the activation term in the equation for s during this continuation; notice that the restriction  $v \leq 0$  is not satisfied everywhere along these computed canard orbits, so that their interpretation in the context of MMOs is not straightforward. The continuation branch undergoes three folds, at  $\varepsilon \approx 0.0385$ ,  $\varepsilon \approx 0.0363$  and  $\varepsilon \approx 0.0412$ , respectively; panels (d1) and (d2) show two coexisting canard orbits for  $\varepsilon = 0.037$ on either side of the first fold, and panels (d3) and (d4)show coexisting canard orbits for  $\varepsilon = 0.04$  on either side of the third fold. Note that the transition across the third fold has the effect that  $\xi_5$  transforms into a canard orbit with only four oscillations; such transitions have been observed in other systems as well [29]. Figure 3(d3) indicates that any trajectory of system (5) that starts on  $S^a_{\varepsilon}$  near a solution on the branch segment in between the second and third fold would exhibit only one small-amplitude oscillation before producing (possibly more than) one action potential (when v becomes positive).

#### V. TRAVELING WAVES OF PDES

In many applications, localized traveling waves play an important role: they may, for instance, represent action potentials that propagate in a neuronal axon, light blips that travel through an optical fiber, or solitary water waves in a channel. Instead of describing the most general type of PDE models, we focus here on systems of reaction-diffusion equations of the form

$$u_t = Du_{xx} + f(u), \tag{6}$$

where  $x \in \mathbb{R}$ ,  $u \in X = C^0(\mathbb{R}, \mathbb{R}^n)$ , and D is a nonnegative diagonal diffusion matrix. Traveling waves are solutions of the form

$$u(x,t) = v(x-ct),\tag{7}$$

where v = v(z) describes the profile, and c is the selected wave speed. Substituting this ansatz into (6), we see that traveling-wave profiles satisfy the ODE

$$Dv_{zz} + cv_z + f(v) = 0,$$
 (8)

where the wave speed c enters as a free parameter. We can rewrite (8) as the first-order system

$$V_z = F(V, c) \tag{9}$$

and use dynamical-systems methods to analyze it. If f(0) = 0, we can seek localized traveling waves of (6) with profiles v(z) that converge to zero exponentially as  $|z| \to \infty$ . Localized traveling waves correspond, therefore, to homoclinic orbits V(z) of (9) that lie in the intersection of the stable and unstable manifolds of the equilibrium V = 0. Without additional structure in the underlying ODE, homoclinic orbits arise as codimension-one phenomena: the wave speed c supplies a free parameter, which suggests that localized traveling waves arise for a discrete set of wave speeds c. Under appropriate genericity conditions, Melnikov theory [11] shows that the stable and unstable manifolds of V = 0will unfold transversally along a homoclinic orbit  $V_*(z)$ upon changing c near the selected wave speed  $c_*$ , provided

$$M := \int_{\mathbb{R}} \langle \psi(z), F_c(V_*(z)) \rangle dz \neq 0, \qquad (10)$$

where  $\psi(z)$  is the unique nontrivial bounded solution of the adjoint variational equation

$$W_z = -F_V(V_*(z))^* W_z$$

Localized traveling waves of (6), which are also referred to as pulses, can be found as homoclinic orbits of the associated traveling-wave ODE (9). Constructing homoclinic orbits is a challenging problem that can often be addressed only through numerical computation. However, when an additional slow-fast structure is present, geometric singular perturbation theory provides a very effective tool to construct pulses. Once a pulse has been identified, homoclinic bifurcation theory can be used to study whether this localized traveling wave can give rise to multi-pulse solutions, which are traveling waves with profiles that resemble several wellseparated copies of the original pulse; these travel at wave speeds close to that of the original pulse.

Once the existence of a pulse  $v_*(z)$  with wave speed  $c_*$  has been shown, one may want to determine whether the resulting solution  $u(x,t) = v_*(x - c_*t)$  is stable as

FIG. 4. (a) Stationary solutions of the PDE (11) are oneparameter families that depend on the location of their center of mass. (b) The spectrum  $\sigma(\mathcal{L}_*)$  of a stable localized traveling wave.

a solution of the original PDE (6). A typical approach consists of transforming (6) into the moving coordinate frame  $(z,t) = (x - c_*t, t)$  to get

$$u_t = Du_{zz} + c_* u_z + f(u), \tag{11}$$

which admits the stationary solution  $u(z,t) = v_*(z)$ . Linearizing this PDE about  $v_*$ , we obtain the linearized operator

$$\mathcal{L}_* u := (D\partial_{zz}^2 + c_*\partial_z + f_u(v_*(z)))u.$$
(12)

The operator  $\mathcal{L}_*$  can be viewed as an unbounded, densely defined, closed operator on  $X = C_{\text{unif}}^0$ : its spectrum on this space provides the necessary information that can be used to prove linear and nonlinear asymptotic stability of the traveling wave  $u(z,t) = v_*(z)$ . We now review some key features of the spectrum of  $\mathcal{L}$ . First,  $\lambda = 0$  always belongs to the spectrum since  $\mathcal{L}_* v'_*(z) = 0$ , and the derivative of the pulse, therefore, provides an eigenfunction associated with  $\lambda = 0$ . Figure 4(a) illustrates the one-parameter family  $v_*(\cdot - p)$ of stationary solutions that is provided by a pulse  $v_*(z)$ via translation of the center of mass to any location  $p \in \mathbb{R}$ . Second, since the pulse profile  $v_*(z)$  converges to zero as  $|z| \to \infty$ , it can be shown that any element in the spectrum of the asymptotic operator

$$\mathcal{L}_0 u := \left( D\partial_z^2 + c_* \partial_z + f_u(0) \right) u \tag{13}$$

that is associated with the rest state u = 0 also lies in the spectrum of  $\mathcal{L}_*$ . The spectrum of  $\mathcal{L}_0$  can be determined via Fourier transform: indeed, the spectrum  $\mathcal{S}_0$  of  $\mathcal{L}_0$  is given by

$$S_0 = \{\lambda \in \mathbb{C} \mid \text{for some } k \in \mathbb{R}, \\ \det \left[ -Dk^2 + i \, k \, c_* + f_u(0) - \lambda \right] = 0 \}.$$
(14)

This set consists of curve segments in the complex plane. If  $S_0$  intersects the open right-half plane, the pulse will be unstable. Therefore, we assume from now on that  $S_0$  lies in the open left-half plane (as the border case where the spectrum of the rest state touches the imaginary axis will result in bifurcations[30, 31]): in this case, the spectrum of  $\mathcal{L}_*$  in the closed right-half plane consists of discrete isolated eigenvalues of finite multiplicity, as is illustrated in Fig. 4(b).

We say that the pulse  $v_*$  is spectrally stable if  $S_0$ lies in the open left-half plane, the eigenvalue  $\lambda = 0$ of  $\mathcal{L}_*$  is simple, and  $\mathcal{L}_*$  has no other eigenvalues with positive real part. A typical stability result consists of the statement that spectral stability of  $\mathcal{L}_*$  implies nonlinear stability with asymptotic phase of the travelingwave family  $\{v_*(\cdot - p); p \in \mathbb{R}\}$ . This result reduces the question of nonlinear stability to studying spectral stability of  $\mathcal{L}_*$ . If we take the view that the set  $S_0$  can, in principle, be calculated case by case, as it involves only an algebraic problem, then it remains to (i) find conditions that guarantee that  $\lambda = 0$  is simple and (ii) identify any other unstable eigenvalues of  $\mathcal{L}_*$ .

To analyze (i), we note that the equation  $\mathcal{L}_* v = 0$  is equivalent to solving the variational equation

$$V_z = F_V(V_*(z), c_*)V$$

of the traveling-wave ODE (9) around the homoclinic orbit  $V_*(z)$  associated with the pulse  $v_*(z)$ . In particular, the condition that the null space of  $\mathcal{L}_*$  is one dimensional ( $\lambda = 0$  has geometric multiplicity one) is equivalent to the condition that the tangent spaces of the stable and unstable manifolds at  $V_*(z)$  intersect in the one-dimensional space spanned by  $V'_*(z)$ . Furthermore, if the geometric multiplicity of  $\lambda = 0$  is one, then its algebraic multiplicity will be one if, and only if, the Melnikov integral M defined in (10) is not zero: indeed, it can be shown that the adjoint solution  $\psi(z)$  is related to the adjoint eigenfunction of the adjoint operator  $\mathcal{L}^*_*$ . This result provides an interesting link between the traveling-wave ODE and stability properties of the PDE linearization.

Regarding property (ii), we can write the eigenvalue problem

$$\mathcal{L}_* u = \lambda u$$

as an equivalent system of linear ODEs of the form

$$V_z = F_V(V_*(z), c_*)V + \lambda BV \tag{15}$$

with parameter  $\lambda$ . A complex number  $\lambda$  is an isolated eigenvalue of  $\mathcal{L}_*$  if, and only if, (15) has a nonzero localized solution, that is, a 'homoclinic orbit'. In other words, if we denote by  $E^s(\lambda)$  and  $E^u(\lambda)$  the linear subspaces of initial conditions of (15) at z = 0 that converge to zero as  $z \to \infty$  and  $z \to -\infty$ , respectively, then we need that these subspaces have a nontrivial intersection. Thus, choosing bases in these subspaces and calculating their determinant, we see that  $\lambda$  is an eigenvalue if, and only if, this determinant, a Wronskian of appropriate solutions of (15), vanishes. This determinant, viewed as a function  $D(\lambda)$  of  $\lambda$ , is referred to as the Evans function [32]: it is analytic in  $\lambda$  for  $\lambda$  to the right of  $S_0$ , and its roots correspond to the sought eigenvalues; in fact, the multiplicity of roots of  $D(\lambda)$  agrees with the algebraic multiplicity of  $\lambda$  viewed as an eigenvalue of  $\mathcal{L}_*$ .

# A. Traveling waves of the FitzHugh–Nagumo equation

To conclude this review, we illustrate the importance of invariant manifolds in both the theoretical and numerical analysis of dynamical systems by considering a model that exhibits all types of invariant manifolds discussed in this paper. More specifically, we consider traveling waves of a FitzHugh–Nagumo model, which have spatial profiles that are homoclinic solutions of the three-dimensional vector field

$$\begin{cases} \varepsilon \dot{x}_{1} = x_{2}, \\ \varepsilon \dot{x}_{2} = \frac{1}{5} [s x_{2} - \\ x_{1} (x_{1} - 1) (\frac{1}{10} - x_{1}) + y - p], \\ \dot{y} = \frac{1}{s} (x_{1} - y). \end{cases}$$
(16)

The geometry of the homoclinic orbits of this system is organized by its invariant manifolds. Study of this problem motivated Jones and Kopell [33] to formulate a general result, the *Exchange Lemma*, that was used to prove existence of a homoclinic orbit of (16) for particular wave speeds given by the parameter s. However, the homoclinic orbit was computed accurately only recently, via intersections of several different types of invariant manifolds [34].

System (16) is a *slow-fast* vector field with one slow variable y and two fast variables  $x_1$  and  $x_2$ . The critical manifold S, defined by  $\{x_2 = 0, y = x_1(x_1 - 1)(0.1 - x_1) + p\}$ , is one dimensional and splits into left, middle and right branches, denoted  $S_l$ ,  $S_m$ , and  $S_r$ , respectively: the inner branch  $S_m$  consists of sources and the two outer branches  $S_l$  and  $S_r$  are saddle equilibria of the layer equations. System (16) has an equilibrium  $\mathbf{q}$ that lies on the critical manifold and additionally solves  $y = x_1$ . The stability of  $\mathbf{q}$  depends upon both p and s. Figure 5(a) shows a bifurcation diagram in the (p, s)plane. The equilibrium  $\mathbf{q}$  undergoes a Hopf bifurcation along the U-shaped curve and homoclinic orbits to  $\mathbf{q}$ are found along the C-shaped curve, where  $q \in S_l$ .

Approximations of the homoclinic orbits for small  $\varepsilon > 0$  can be pieced together from the singular limit. Beginning at  $q \in S_l$ , the first segment of the homoclinic orbit follows the unstable manifold of  $\mathbf{q}$  in the layer equations to the layer equilibrium on  $S_r$  with the same  $(x_1, x_2)$ -coordinates as  $\mathbf{q}$ . As described by the Exchange Lemma, the trajectory then turns and follows  $S_r$  to a value of the slow variable y where there is a connecting orbit that returns from  $S_r$  to  $S_l$ ; the connecting orbit then follows  $S_l$  back to  $\mathbf{q}$ .



FIG. 5. (a) Bifurcation diagram of traveling waves for system (16) in the (p, s)-plane consisting of a U-shaped (blue) curve of Hopf bifurcations and a C-shaped (red) curve of homoclinic bifurcations; the dashed curves are their singular limit as  $\varepsilon \to 0$ . (b) Traveling-wave homoclinic orbit (red curve) to the saddle **q** with slow segments near the critical manifold (blue curve).

Fenichel proved that the critical manifold branches  $S_l$  and  $S_r$  perturb to locally invariant slow manifolds for small  $\varepsilon > 0$ , along with their stable and unstable manifolds [20]. Hence, the slow-fast decomposition of the homoclinic orbits persists when  $\varepsilon > 0$ ; however, as a heteroclinic connection between saddles, it occurs for parameters that lie on a curve in the (p, s)-plane. It is difficult to compute the homoclinic orbits because the relevant slow manifolds are saddle like in the fast directions. Numerical solutions of initial value problems that start on or close to these manifolds can only follow them for times that are O(1) with respect to the fast timescale. Guckenheimer and Kuehn [34] developed a two-point boundary value problem and associated solver that locates these manifolds. The directions of its stable and unstable manifolds were estimated as well, yielding initial conditions for computing trajectories on these manifolds with initial value solvers; see Sec. VI for the details of these calculations. This approach allows for the computation of the whole homoclinic orbit as a composite of its slow and fast segments, each computed separately and matched together at the respective endpoints. The full homoclinic orbit to  $\mathbf{q}$  is illustrated in Fig. 5(b).

Champneys et al. noted that the 'CU' bifurcation diagram shown in Fig. 5(a) is puzzling [35]. They report that the curve of homoclinic bifurcations appears to end without contacting another more degenerate bifurcation. Further analysis of invariant manifolds resolved this enigma [34]. The clue to the discrepancy is that  $\mathbf{q}$  may undergo a *subcritical* Hopf bifurcation, after which it no longer lies on  $S_l$ . There is a family of periodic orbits emerging from  $\mathbf{q}$  which bounds its stable manifold. A consequence is that there is no way for trajectories following the slow manifold associated with  $S_l$  to reach **q** for parameters that are close to the Hopf curve. The stable manifold of  $\mathbf{q}$  and the unstable manifold of the saddle slow manifold do not intersect. However, as the parameters move farther from the Hopf curve, the stable manifold of the equilibrium begins to spiral around the periodic orbit created at the Hopf bifurcation. It then passes through a tangency with the unstable manifold of the slow manifold  $S_l$  followed by transversal intersections of the two manifolds; see Fig. 3 in Ref. [34]. The tangency of these manifolds can be regarded as another codimension-one bifurcation that occurs along a curve in the (p, s)-plane. Because this tangency is independent of the connection from  $\mathbf{q}$  to the saddle slow manifold associated with  $S_r$ , the associated two bifurcation curves cross transversally, intersecting at the end of the C-curve of homoclinic bifurcations. We refer to Ref. [34] for more detail on the exponentially small scales found in the folding of the C-curve.

This example illustrates that invariant manifolds of different kinds and their intersections play a prominent role in shaping the dynamics of slow-fast vector fields. Homoclinic tangency of stable and unstable manifolds of periodic orbits has long been a focus of the analysis of horseshoes and their bifurcations, but the phenomenology associated with the homoclinic orbits of the FitzHugh–Nagumo model have been a new development. Similarly, intersections between a repelling slow manifold and the unstable manifold of a saddle equilibrium are important in mixed-mode oscillations of the Koper model [13, 36], and the tangency of these manifolds demarcates part of a parameter-space boundary for these complex oscillations; see also Ref. [19]. In a broader context, we know relatively little about *global* returns of systems with multiple timescales; i.e., dynamics that lead to recurrence of trajectories to specific regions of a phase space following large excursions from these regions. We even lack a sharp formulation of mathematical problems and conjectures that generalize the observations made in examples of three-dimensional slow-fast systems.

#### VI. NUMERICAL METHODS FOR MANIFOLDS

Equilibria, periodic orbits and their local bifurcations can be found with standard dynamical systems software such as AUTO [16], MATCONT [37] and COCO [38]. Here periodic orbits are computed as solutions to a boundary value problem (BVP) with periodic boundary conditions and an appropriate phase condition. More generally, the integrated boundary value solvers of the above packages locate an orbit segment  $\mathbf{u}(t)$  with  $t \in [0, 1]$  that satisfies the time-rescaled equation

$$\dot{\mathbf{u}} = T f(\mathbf{u}),$$

subject to specified boundary conditions, where T is the integration time (which may be negative) associated with the normalized orbit segment **u**. The solution of the BVP is found with the method of collocation as a piecewise polynomial over a specified mesh. A first periodic solution can be constructed near a Hopf bifurcation or, when it is stable, found by numerical integration.

An approximate homoclinic or heteroclinic orbit can be found and continued as an orbit segment whose end points lie in the stable and unstable linear eigenspaces near the respective equilibrium; one speaks of projection boundary conditions [39]. To find an initial orbit segment **u** satisfying this BVP one can consider a periodic orbit of high period, or perform what is known as a homotopy step as implemented in the toolbox HOM-CONT [15] that is part of the package AUTO; also supplied are test functions that allow the user to identify certain codimension-two global bifurcations, including inclination and orbit flips.

Several methods have been developed for computing invariant manifolds of dimension higher than one, with emphasis on two-dimensional stable and unstable manifolds of equilibria in  $\mathbb{R}^3$ ; see the survey Ref. [40]. We concentrate here on the general idea to select a region of interest and define the two-dimensional (invariant) manifold in this region as a one-parameter family of orbit segments, defined by a suitable BVP. A review of this approach can be found in Ref. [41]; for more general background information on continuation methods see Ref. [42].

Restricting our discussion to three-dimensional systems for simplicity, we consider an orbit segment  $\mathbf{u}$  with one end point on a one-dimensional curve (for example, a line) and the other on a two-dimensional surface (for example a planar section). This two-point boundary value problem setup is very flexible, and the boundary conditions on either end point can be formulated implicitly; for example, one can also consider orbit segments of a fixed integration time or specified fixed arclength; see Refs. [41] and [40].

Figure 6(a) shows the computational setup for the repelling slow manifold of system (5) in Fig. 3(b). Here,



FIG. 6. Illustration of BVP setup for computing families of orbit segments. (a) An initial orbit segment **u** of system (5) with  $\mathbf{u}(0) \in L^r \subset S^r$  and  $\mathbf{u}(1) \in \Sigma$ ; varying  $\mathbf{u}(0)$  along  $L^r$ produces the repelling slow manifold  $S_{\varepsilon}^r$ ; reproduced from Ref. [28]. (b) Lin's method setup for a connection between an equilibrium **p** and a periodic orbit  $\Gamma$ , consisting of two orbit segments,  $Q^-$  from **p** and  $Q^+$  from  $\Gamma$ , that end in a section  $\Sigma$  along a specified Lin direction Z; from Ref. [43, Fig. 1(a)]. ©2008 IOP Publishing & London Mathematical Society. Reproduced with permission. All rights reserved.

 $\mathbf{u}(0)$  is restricted to the line denoted  $L^r \subset S^r$  with v = 0, and  $\mathbf{u}(1)$  is restricted to the plane  $\Sigma$  that is perpendicular to the fold curve F and contains the foldednode singularity. To obtain such an orbit segment we perform two homotopy steps [28]. The orbit segment  $\mathbf{u}$  shown in Fig. 6(a) with associated integration time T is an isolated solution of a solution family that is parametrized by the point  $\mathbf{u}(0)$  on the line  $L^r = L^r(\theta)$ . Continuation in the parameter  $\theta$  then produces the repelling slow manifold  $S_{\varepsilon}^r$  as a surface.

In order to find more complicated connecting orbits it may be useful to split the orbit into several segments, each to be computed with a BVP solver. In particular, this approach is used in implementations of what is known as Lin's method [44, 45]. The underlying idea is to compute pairs of orbit segments (with associated integration times) in such a way that their end points are constrained to lie along a specified vector direction on a common surface defining one of the boundary conditions for these segments. Lin's method has been implemented for the detection of multipulse homoclinic orbits [46], and for so-called EtoP connections between equilibria and periodic orbits [43] and PtoP connections between periodic orbits [47].

Figure 6(b) shows the Lin's method setup for the computation of a codimension-one EtoP connection between a saddle equilibrium  $\mathbf{p}$  and a saddle periodic orbit  $\Gamma.$  The orbit segment  $Q^-$  starts from a point on the unstable eigenvector  $\mathbf{v}^u$  of  $\mathbf{p}$  and ends in the section  $\Sigma$ ; similarly the orbit segment  $Q^+$  starts from  $\Sigma$  to a point on the vector  $\mathbf{v}^s$  in the unstable bundle of  $\Gamma$ . The two end points of  $Q^-$  and  $Q^+$  in  $\Sigma$  lie along the Lin direction Z, which can be chosen freely provided a mild genericity condition is satisfied. The signed difference between the two end points along the fixed direction Z is a well-defined test function that is referred to as the Lin gap; continuation in a system parameter, while keeping Z fixed, can then be used to find a zero of the Lin gap, which corresponds to the sought connecting orbit.

A similar strategy was used in calculating the homoclinic orbit of system (16), but a customized boundary value solver was developed to compute the slow segments of this orbit. The homoclinic orbit is split into four segments, two that follow the slow manifolds  $S_r$ and  $S_l$ , one that connects the equilibrium **q** to  $S_r$  and a fourth that connects  $S_r$  to  $S_l$ . The connection from **q** to  $S_r$  is the part of the homoclinic orbit that exists for only a discrete value of the wave-speed parameter s. The first step in finding the homoclinic orbit is to compute this segment by a shooting algorithm that uses initial conditions on the linear approximation of the one-dimensional manifold  $W^{u}(q)$ , for different values of the wave speed s. The value of s for which this connection is found is then fixed in the remainder of the calculations of the homoclinic orbit. Note that, since  $S_r$  is normally hyperbolic, it is easy to determine which direction  $W^u(q)$  turns as it approaches  $S_r$ .

The next step in finding the homoclinic orbit is to calculate accurate approximations to  $S_r$  and  $S_l$  with a boundary value solver. Figure 7(a) illustrates the setup of the two-point boundary value problem used to calculate  $S_r$ . In making the calculation well conditioned, it is important to choose boundary conditions that make a large angle with the vector field in an entire region of the boundary manifold. Thus, instead of just computing the segment along the slow manifold where the direction of the vector field changes rapidly, the boundary conditions are located transverse to the stable and unstable manifolds of  $S_r$ , as illustrated by the line seg-



FIG. 7. (a) Boundary value problem setup from  $B_l$  to  $B_r$  for the computation of slow manifold  $S_r$  of saddle type of (16) for p = 0, s = 1.2463 and  $\varepsilon = 0.001$ . (b) Associated heteroclinic connection of slow manifolds: ten blue trajectories starting along  $S_r$  are computed forward to a cross-section  $\Sigma$ defined by  $x_1 = 0.5$ , and ten red trajectories starting on  $S_l$ are computed backward to  $\Sigma$ . It is apparent In  $\Sigma$  that the unstable manifold of  $S^r$  intersects the stable manifold of  $S^l$ transversally.

ment  $B_r$  and rectangle  $B_l$  in Fig. 7(a). The (time) length of the trajectory is chosen so that the algorithm computes longer segments of  $S_r$  and  $S_l$  than those that are part of the homoclinic orbit.

The directions of the stable and unstable manifolds along  $S_r$  and  $S_l$  were estimated by the linearization of the fast (layer) equations along the slow manifold; an initial value solver was used to 'sweep' out the manifolds by computing sets of trajectories whose initial conditions were constructed from the linearization. Figure 7(b) shows some of these trajectories as well as the surfaces of the stable and unstable manifolds interpolated from these. These integrations were terminated on a common plane to illustrate the transversality of their intersection along the fast segment of the heteroclinic orbit that connects  $S_r$  to  $S_l$ . The Exchange Lemma describes important aspects of the geometry of this connection.

The matching conditions of the four segments of the homoclinic orbit are more or less automatic from the normal hyperbolicity of the slow manifolds. The slow segments of the homoclinic orbit orbit must lie exponentially close to the slow manifolds  $S_r$  to  $S_l$ , so they cannot be distinguished from these manifolds numerically. Thus, the errors associated with using approximate boundary conditions that place the endpoints of the segments on the stable and unstable manifolds of  $S_r$ to  $S_l$  cannot be resolved without heroic computations of extreme precision. The continuity of the invariant manifolds with respect to perturbations of the vector field and their transversal intersections on the boundaries of the cross-sections used in the phase space extended with the parameter s make us confident that the numerically computed trajectory is an excellent approximation to the homoclinic orbit.

#### VII. DISCUSSION

This short review attempted to highlight some recent examples of how the study of global invariant manifolds and their bifurcations can help unravel the overall dynamics of a given system. The examples are by no means exhaustive, but we hope that they convey the usefulness of this approach and the associated advanced numerical methods. Indeed, invariant manifolds of different kinds are also key ingredients in the dynamics of numerous other systems, and quite a number of challenges remain. We mention a few of them briefly.

- The study of invariant manifolds near the more complicated cases B and C of codimension-two homoclinic flip orbits is the subject of ongoing research; here also (possibly infinitely many) periodic orbits of saddle type play a role as well.
- The study of invariant manifolds near heteroclinic cycles or chains involving equilibria and periodic orbits is a promising direction for future research.
- The examples in this paper all involve invariant manifolds of dimensions one and two in threedimensional vector fields. There is a robust literature on identifying attracting slow manifolds in systems of chemical reactions, especially in the context of combustion [48], and this appears to be an area ready for further development. Computing stable manifolds of low codimension in high-

dimensional systems is one strategy to identify attractor basin boundaries in high-dimensional systems [49].

- Higher-dimensional compact invariant objects, such as invariant tori, are also of great interest in many areas of application, and computing them and their stable and unstable manifolds is an active area of research [50–53] not touched upon in this review.
- Dynamical systems with symmetries, conserved quantities or network structure appear in many applications. Invariant manifolds are perhaps even more important as key ingredients in the

analysis of such systems, but adjustments of the numerical methods to take account of these structures is needed [54]. Beyond manifolds, more geometric objects with singularities arise in these settings. Group theoretical methods are a powerful tool for the analysis of systems with symmetry [55].

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