



COMPUTER TOOLS FOR BIFURCATION ANALYSIS: GENERAL APPROACH WITH APPLICATION TO DYNAMICAL AND DISTRIBUTED SYSTEMS

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A general approach of the automated algorithms for derivation of amplitude equations for dynamical and distributed systems is presented. A brief description of the *Mathematica* functions designed using this approach is given. Application of the functions is illustrated by several examples dealing with dynamical and distributed systems.

1. Introduction	984
2. Bifurcations of Dynamical Systems	986
2.1. Multiscale Expansion	986
2.2. Monotonic Bifurcation	987
2.2.1 Fold Bifurcation	987
2.2.2 Transcritical Bifurcation	987
2.2.3 Higher-Order Bifurcations	988
2.3. Hopf Bifurcation	988
2.4. Automated Generation of Normal Forms	990
2.5. Computation of Coefficients	992
2.5.1 Function CalculateCoefficient	992
2.5.2 Lorenz Model	992
2.5.3 Brusselator Model	992
2.5.4 Exothermic Reaction in a Stirred Tank Reactor	993
3. General Algorithm for Distributed Systems	995
3.1. Introduction	995
3.2. Linear Analysis and Dispersion Relation	996
3.3. Multiscale Expansion	996
3.4. Function BifurcationTheory	997
4. Amplitude Equations for Reaction–Diffusion Problems	998
4.1. Long-Scale Instabilities	998
4.2. Turing Bifurcation	999
4.2.1 Hopf Bifurcation	1000

4.3.	Brusselator Model	1000
4.3.1	Monotonic Bifurcation	1000
4.3.2	Oscillatory Bifurcation	1001
4.4.	Two-Level Laser Model	1001
4.4.1	Oscillatory Bifurcation	1001
5.	Amplitude Equations for Convective Problems	1002
5.1.	Convective Instabilities	1002
6.	Resonant and Degenerate Cases	1003
6.1.	Three-Wave Resonance in Turing Bifurcation	1003
6.1.1	General Results	1003
6.1.2	Calculations for Brusselator Model	1004
6.2.	Four-Wave Resonance in Oscillatory Instability	1005
6.3.	Algebraic Degeneracy — Hopf–Turing Bifurcation	1005
A	Linear Analysis and Amplitude Equations for Lorenz Model	1006
B	Linear Analysis for Brusselator Model	1007

1. Introduction

Amplitude equations describe behavior of evolutionary systems in the vicinity of threshold, or critical values of parameters that mark a point of qualitative change in behavior, like a transition from a quiescent state to convection, or from rigid mechanical equilibrium to vibration, or from a homogeneous to patterned state of a material medium. Near the criticality, the behavior of systems of different physical origin is described by representative equations belonging to one of the universal classes that are determined by the character of the transition.

A common procedure of derivation of amplitude equations starts from a certain system of evolution equations symmetric to spatial translations and rotations and time translations; a necessary condition is that it does not include explicit dependence on spatial coordinates and time. This underlying system may be, in the order of ascending complexity, a *dynamical* system (autonomous ODEs), an autonomous *distributed* system described by PDEs but not restricted by boundary conditions, and a distributed system with *vertical structure* constrained by boundary conditions along some spatial coordinates but retaining translational symmetry in other (unconstrained) directions. A solution that retains all symmetries of the underlying system is called a *basic state*. This state may become unstable to infinitesimal perturbations in a certain parametric domain. The instability may be connected with the

emergence of new solutions with a more complicated spatiotemporal structure.

In dynamical systems, possible transitions are bifurcation of multiple stationary states (monotonic bifurcation) or transition to oscillatory behavior (Hopf bifurcation). If the phase trajectory of the dynamical system remains in the vicinity of the basic state even after the latter becomes unstable, it can be replaced there by certain reduced equations called *normal forms* [Guckenheimer & Holmes, 1983; Hale & Koçak, 1991]. In distributed systems there are two more possibilities: transition to a stationary pattern (*Turing* bifurcation) or to a wave pattern (Hopf bifurcation at nonzero wavenumber). Like normal forms of dynamical systems, amplitude equations describe behavior in the vicinity of the basic state; they may include, however, also differential terms describing spatial inhomogeneities on an extended scale or spatial modulation of a primary pattern.

There is a number of celebrated “universal” equations which have been extensively studied in physical literature. The general structure of these equations can be often predicted by symmetry considerations. Some of them were first suggested as models, others were derived as rational approximations in a certain physical context, and then discovered again in apparently unrelated problems. Although these equations, strictly speaking, may be valid only in a very limited parametric domain, they retain a variety of dynamic behavior due to a high

parametric sensitivity in the vicinity of a transition point. Parametric boundaries between regions of qualitatively different dynamic behavior can be drawn as relations between coefficients of amplitude equations or normal forms. If these coefficients, in their turn, are expressed through measurable physical parameters, the boundaries can be mapped upon the actual parameter space, and then further continued into a region where universal equations are no longer valid quantitatively but still faithfully describe qualitative features of behavior of a complex nonlinear system.

It is important therefore not only to be able to predict a general form of amplitude equations or normal forms appropriate to different kinds of bifurcations but to have at hand reliable tools for actual computation of their coefficients, starting with specific underlying evolution equations. The applicable algorithms, known as *center manifold* methods in mathematical literature [Guckenheimer & Holmes, 1983; Hale & Koçak, 1991], or elimination of “slaved” variables in physical literature [Haken, 1987], are well established, at least in standard cases. Actual computations are, however, repetitive and time-consuming, and have been carried out in scientific literature on a case-to-case basis. Only very rarely can they be done manually by anybody lacking Leverrier’s patience. Application of modern computer algebra systems — first, REDUCE and MACSYMA, and later, MAPLE and *Mathematica* — is an obvious remedy. It is difficult to estimate, to what extent they are used nowadays for the study of specific bifurcation problems, as it is not always explicitly acknowledged in resulting publications. A case-to-case application is, however, still arduous and inefficient, compared to the realization of a general algorithm.

A MACSYMA-based (not fully automated) algorithm for derivation of normal forms of dynamical systems has been written by Rand and Armbruster [1987]. Another well-known bifurcation analysis package AUTO by Doedel, as well as the algorithm by Guckenheimer *et al.* [1997] for the analysis of Hopf bifurcation, are restricted to numerical tracking of solutions of dynamical systems. No general computer-aided algorithms have been suggested so far, to the best of the authors’ knowledge, for the analysis of bifurcations in distributed systems.

This tutorial review describes a *Mathematica*-based automated algorithm for the derivation of amplitude equations for both dynamical and distributed systems in either symbolic or numerical

form. The algorithm makes use of *Mathematica* capabilities as a *programming language* [Wolfram, 1991, 1996] that allows to define special *functions* carrying out complicated tasks in response to simple and well-defined inputs.

In the course of our work on this algorithm, we arrived at the conclusion that computations are most efficient, in terms of CPU time and computer resources, when any specific bifurcation problem is approached as a part of a broader class of problems leading to an amplitude equation of the same structure. Accordingly, all computations are carried out in two stages. The general algorithm based on multiscale bifurcation expansion is implemented by the function `BifurcationTheory`. The input of this function must be given in a generalized form, without specifying particular nonlinear functions, eigenvectors, etc. The underlying system should be defined as a single operator equation where various vectors or arrays are denoted by symbols rather than being specified explicitly. The output depends therefore only on the type of the bifurcation, applicable symmetries and the desired order of expansion. It includes the amplitude equation and unresolved expressions for its coefficients, written in a generalized symbolic form and containing unimplemented inverse operators.

The next stage is the actual computation implemented by the function `CalculateCoefficient`. It takes the necessary data for a specific system and uses them in the output of `BifurcationTheory` to produce either explicit symbolic expressions for coefficients or their numerical values. Thus, the program works much in the way as an intelligent mathematician would: first preparing general formulae and then working out a specific example. This gives an order of magnitude acceleration compared to an earlier version of our algorithm [Pismen *et al.*, 1996] where amplitude equations containing explicit expressions for coefficients were computed directly for specific problems.

The paper is organized as follows. Although one and the same internal algorithm works for dynamic and distributed systems, we start, for pedagogical reasons, with a detailed treatment of dynamical systems in Sec. 2. First, the general algorithm based on multiscale bifurcation expansion is outlined, and then the function `BifurcationTheory` designed to implement this algorithm is introduced and applied to both monotonic and Hopf bifurcations. This is followed by specific examples.

Starting from Sec. 3, we repeat the same scheme for distributed systems. The general algorithm is outlined in Sec. 3 for a problem written in the most general nonlinear operator form. In Sec. 4, the function `BifurcationTheory` is applied to reaction–diffusion problems, followed by specific examples of computation of coefficients.

In Sec. 5, we consider along the same lines some problems involving convection that cannot be reduced to a reaction–diffusion form. Resonant and algebraically degenerate cases are discussed in Sec. 6. The primary cause of degeneracy in distributed systems with two unrestrained direction is rotational symmetry that makes excitation of stationary inhomogeneities or waves with different directions of the wavenumber vector. Strong resonances may involve in such systems three waveforms in the case of a monotonic (Turing), and four waveforms in the case of a wave (Hopf) bifurcation. We shall also give an example of a parametric (“accidental”) degeneracy involving mixed Hopf and Turing modes. The algorithm is applicable only when the degeneracy is algebraic but not geometric. The latter case requires essential modification of the multiscale expansion procedure, and is outside the scope of this communication.

2. Bifurcations of Dynamical Systems

2.1. Multiscale expansion

The standard general algorithm for derivation of amplitude equations (normal forms) is based on *multiscale expansion* of an underlying dynamical system in the vicinity of a bifurcation point. Consider a set of first-order ordinary differential equations in \mathbb{R}^n :

$$d\mathbf{u}/dt = \mathbf{f}(\mathbf{u}, \mathbf{R}), \quad (1)$$

where $\mathbf{f}(\mathbf{u}; \mathbf{R})$ is a real-valued n -dimensional vector-function of an n -dimensional array of dynamic variables \mathbf{u} , that is also dependent on an m -dimensional array of parameters \mathbf{R} . We expand both variables and parameters in powers of a dummy small parameter ε :

$$\begin{aligned} \mathbf{u} &= \mathbf{u}_0 + \varepsilon\mathbf{u}_1 + \varepsilon^2\mathbf{u}_2 + \dots, \\ \mathbf{R} &= \mathbf{R}_0 + \varepsilon\mathbf{R}_1 + \varepsilon^2\mathbf{R}_2 + \dots \end{aligned} \quad (2)$$

Next, we introduce a hierarchy of time scales t_k rescaled by the factor ε^k , thereby replacing the function $\mathbf{u}(t)$ by a function of an array of rescaled time

variables. Accordingly, the time derivative is expanded in a series of *partial* derivatives $\partial_k \equiv \partial/\partial t_k$:

$$\frac{d}{dt} = \partial_0 + \varepsilon\partial_1 + \varepsilon^2\partial_2 + \dots \quad (3)$$

Let $\mathbf{u} = \mathbf{u}_0(\mathbf{R}_0)$ be an equilibrium (a fixed point) of the dynamical system (1), i.e. a zero of the vector-function $\mathbf{f}(\mathbf{u}; \mathbf{R})$ at a point $\mathbf{R} = \mathbf{R}_0$ in the parametric space. The function $\mathbf{f}(\mathbf{u}; \mathbf{R})$ can be expanded in the vicinity of $\mathbf{u}_0, \mathbf{R}_0$ in Taylor series in both variables and parameters:

$$\begin{aligned} \mathbf{f}(\mathbf{u}; \mathbf{R}) &= \mathbf{f}_{\mathbf{u}}(\mathbf{u} - \mathbf{u}_0) + \frac{1}{2}\mathbf{f}_{\mathbf{uu}}(\mathbf{u} - \mathbf{u}_0)^2 \\ &+ \frac{1}{6}\mathbf{f}_{\mathbf{uuu}}(\mathbf{u} - \mathbf{u}_0)^3 + \dots + \mathbf{f}_{\mathbf{R}}(\mathbf{R} - \mathbf{R}_0) \\ &+ \mathbf{f}_{\mathbf{uR}}(\mathbf{u} - \mathbf{u}_0)(\mathbf{R} - \mathbf{R}_0) \\ &+ \frac{1}{2}\mathbf{f}_{\mathbf{uuR}}(\mathbf{u} - \mathbf{u}_0)^2(\mathbf{R} - \mathbf{R}_0) + \dots \end{aligned} \quad (4)$$

The derivatives with respect to both variables and parameters $\mathbf{f}_{\mathbf{u}} = \partial\mathbf{f}/\partial\mathbf{u}$, $\mathbf{f}_{\mathbf{uu}} = \partial^2\mathbf{f}/\partial\mathbf{u}^2$, $\mathbf{f}_{\mathbf{R}} = \partial\mathbf{f}/\partial\mathbf{R}$, $\mathbf{f}_{\mathbf{uR}} = \partial^2\mathbf{f}/\partial\mathbf{u}\partial\mathbf{R}$, etc. are evaluated at $\mathbf{u} = \mathbf{u}_0, \mathbf{R} = \mathbf{R}_0$.

Using Eqs. (2)–(4) in Eq. (1) yields in the first-order

$$\partial_0\mathbf{u}_1 = \mathbf{f}_{\mathbf{u}}\mathbf{u}_1 + \mathbf{f}_{\mathbf{R}}\mathbf{R}_1. \quad (5)$$

The homogeneous linear equation

$$\mathcal{L}\mathbf{u}_1 \equiv (\mathbf{f}_{\mathbf{u}} - \partial/\partial t_0)\mathbf{u}_1 = 0 \quad (6)$$

obtained by setting in Eq. (5) $\mathbf{R}_1 = 0$ governs the stability of the stationary state $\mathbf{u} = \mathbf{u}_0$ to infinitesimal perturbations. The state is stable if all eigenvalues of the Jacobi matrix $\mathbf{f}_{\mathbf{u}}$ have negative real parts. This can be checked with the help of the standard *Mathematica* function `Eigenvalues`. Computation of *all* eigenvalues is, however, superfluous, since stability of a fixed point is determined by the location in the complex plane of a *leading* eigenvalue, i.e. with the largest real part. Generically, the real part of the leading eigenvalue vanishes on a codimension one subspace of the parametric space called a *bifurcation manifold*. The two types of *codimension one* bifurcations that can be located by local (linear) analysis are a *monotonic* bifurcation where a real leading eigenvalue vanishes, and a *Hopf* bifurcation where a leading pair of complex conjugate eigenvalues is purely imaginary. Additional conditions may define bifurcation manifolds of higher codimension.

2.2. Monotonic bifurcation

2.2.1. Fold bifurcation

A monotonic bifurcation is also a bifurcation of equilibria of the dynamical system (1). Setting $\mathbf{u}_1 = \text{const}$, i.e. $\partial_0 \mathbf{u}_1 = 0$, allows to find a shift of the stationary solution due to small variations of parameters

$$\mathbf{u}_1 = -\mathbf{f}_{\mathbf{u}}^{-1} \mathbf{f}_{\mathbf{R}} \mathbf{R}_1. \quad (7)$$

The $n \times m$ array $\mathbf{f}_{\mathbf{u}}^{-1} \mathbf{f}_{\mathbf{R}}$ is recognized as the *parametric sensitivity* matrix. Continuous dependence on parameters can be used to construct a branch of equilibria which *terminates* at a bifurcation point \mathbf{R}_0 .

On a monotonic bifurcation manifold, the matrix $\mathbf{f}_{\mathbf{u}}$ has no inverse. This means that one can neither construct a stationary solution at values of parameters close to this point, nor characterize the stability of the equilibrium in the linear approximation. The dynamics in the vicinity of the bifurcation manifold is governed by a *nonlinear* amplitude equation to be obtained in higher orders of the expansion.

Generically, the zero eigenvalue is nondegenerate. Let \mathbf{U} be the corresponding eigenvector satisfying $\mathbf{f}_{\mathbf{u}} \mathbf{U} = 0$. Then

$$\mathbf{u}_1 = a(t_1, t_2, \dots) \mathbf{U} \quad (8)$$

is the solution of Eq. (6) that remains stationary on the fast time scale t_0 . The amplitude a is so far indeterminate, and can depend on slower time scales.

The inhomogeneous equation (5) has solutions constant on the rapid time scale, provided its inhomogeneity does not project on the eigenvector \mathbf{U} . This condition is

$$\kappa_1 \equiv \mathbf{U}^\dagger \mathbf{f}_{\mathbf{R}} \mathbf{R}_1 = 0, \quad (9)$$

where \mathbf{U}^\dagger is the eigenvector of the *transposed* matrix $\mathbf{f}_{\mathbf{u}}^\dagger = \text{Transpose}[\mathbf{f}_{\mathbf{u}}]$ satisfying $\mathbf{f}_{\mathbf{u}}^\dagger \mathbf{U}^\dagger = 0$; we assume that the eigenvector is normalized: $\mathbf{U}^\dagger \mathbf{U} = 1$. Equation (9) defines the *tangent hyperplane* to the bifurcation manifold at the point $\mathbf{R} = \mathbf{R}_0$.

Before writing up the second-order equation, we require that the second-order deviation \mathbf{u}_2 remain constant on the rapid time scale (otherwise it might outgrow \mathbf{u}_1 at long times). The dependence upon slower time scales must be expressed exclusively through the time dependence of the amplitude a . Using Eq. (8), we write the second-order

equation as

$$\mathbf{f}_{\mathbf{u}} \mathbf{u}_2 = \partial_1 a \mathbf{U} - \mathbf{f}_{\mathbf{R}} \mathbf{R}_2 - a \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_1 - \frac{1}{2} a^2 \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}. \quad (10)$$

The solvability condition of this equation is

$$\partial_1 a = \kappa_2 + \lambda_1 a + \mu_0 a^2. \quad (11)$$

The parameters of Eq. (11) are

$$\begin{aligned} \kappa_2 &= \mathbf{U}^\dagger \mathbf{f}_{\mathbf{R}} \mathbf{R}_2 + \frac{1}{2} \mathbf{U}^\dagger \mathbf{f}_{\mathbf{RR}} \mathbf{R}_1 \mathbf{R}_1, \\ \lambda_1 &= \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_1, \\ \mu_0 &= \frac{1}{2} \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}. \end{aligned} \quad (12)$$

The indices correspond to the scaling of respective parametric deviations from the bifurcation point. In a generic case, one can consider only parametric deviations transverse to the bifurcation manifold, and set $\mathbf{R}_1 = 0$ to satisfy Eq. (9); then $\lambda_1 = 0$, and generic equation for slow dynamics near the bifurcation manifold becomes

$$\partial_1 a = \kappa_2 + \mu_0 a^2. \quad (13)$$

This equation can be also obtained by shifting the amplitude in Eq. (11). On the one side of the bifurcation manifold, where κ_2 has the sign opposite to that of μ_0 , there are two stationary states $a = \pm \sqrt{-\kappa_2/\mu_0}$. When viewed as a solution of Eq. (13), one of them is stable, and the other, unstable. The stable solution corresponds to a stable equilibrium of the original system Eq. (1), provided the rest of eigenvalues of the matrix $\mathbf{f}_{\mathbf{u}}$ have negative real parts. On the other side of the bifurcation manifold, where the signs κ_2 and μ_0 are the same, there are no stationary states. The trajectory of the dynamical system is deflected then to another attractor, far removed from \mathbf{u}_0 . Thus, the system undergoes a *first-order phase transition* when the bifurcation manifold is crossed. If the value of some dynamic variable or other characteristic of the solution is drawn as a function of parameters, the bifurcation locus can be seen as the projection of a fold of the solution manifold on the parametric plane; accordingly, the generic monotonic bifurcation is also called a *fold* bifurcation.

2.2.2. Transcritical bifurcation

It may happen that the matrix $\mathbf{f}_{\mathbf{R}}$ as well the tensor $\mathbf{f}_{\mathbf{RR}}$ vanish identically. This would be the case when \mathbf{u}_0 is a “trivial” solution that remains constant at

all values of parameters. Then Eq. (9) is satisfied identically, and Eq. (11) reduces to

$$\partial_1 a = \lambda_1 a + \mu_0 a^2. \quad (14)$$

This equation has two solutions, $a = 0$ and $a = -\lambda_1/\mu_0$, on both sides of the bifurcation manifold, but the two solutions interchange stability when this manifold is crossed. This bifurcation is called *transcritical*.

2.2.3. Higher-order bifurcations

If $\mu_0 = 0$, the expansion should be continued to the next order. The coefficient μ_0 may vanish identically due to the symmetry of the original problem to inversion of \mathbf{u} . Otherwise, it can be equal to zero at certain values of the parameters of the problem. Generally, the two conditions, $\text{Det}[\mathbf{f}_{\mathbf{u}}] = 0$ and $\mu_0 = 0$ are satisfied simultaneously on a *codimension two* manifold in the parametric space that corresponds to a *cusplike* singularity.

In order to continue the expansion, we restrict parametric deviations in such a way that the dependence on t_1 be suppressed. Deviations *transverse* to the bifurcation manifold have to be restricted by the condition $\kappa_2 = 0$, which is stronger than Eq. (9). First-order parametric deviations \mathbf{R}_1 *parallel* to the bifurcation manifold, which are still allowed by Eq. (9), should be now restricted by the condition $\lambda_1 = 0$. If the array \mathbf{R} contains two parameters only, the conditions $\lambda_1 = 0$ and $\kappa_1 = 0$ imply, in a nondegenerate case, that first-order parametric deviations should vanish identically. When more parameters are available, parametric deviations satisfying both these conditions are superfluous, since they correspond just to gliding into a closer vicinity of another point on the cusp bifurcation manifold in a higher-dimensional parametric space. Further on, we shall set therefore \mathbf{R}_1 to zero identically.

The dynamics unfolding on a still slower time scale t_2 should be determined from the third-order equation

$$\begin{aligned} \mathbf{f}_{\mathbf{u}} \mathbf{u}_3 &= \partial_2 a \mathbf{U} - \mathbf{f}_{\mathbf{R}} \mathbf{R}_3 - a \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_2 \\ &- a \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{u}_2 - \frac{1}{6} a^3 \mathbf{f}_{\mathbf{uuu}} \mathbf{U} \mathbf{U} \mathbf{U}. \end{aligned} \quad (15)$$

The second-order function \mathbf{u}_2 has to be found by solving Eq. (10), now reduced to the form

$$\mathbf{f}_{\mathbf{u}} \mathbf{u}_2 = -\mathbf{f}_{\mathbf{R}} \mathbf{R}_2 - \frac{1}{2} a^2 \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}. \quad (16)$$

Only the solution of the inhomogeneous equation, which does not project on the eigenvector \mathbf{U} , is relevant. It can be expressed as

$$\mathbf{u}_2 = \mathbf{U}_2^{(2)} + a^2 \mathbf{U}_2^{(0)}. \quad (17)$$

The solvability condition of Eq. (15) is obtained then in the form

$$\partial_2 a = \kappa_3 + \lambda_2 a + \nu_0 a^3, \quad (18)$$

where

$$\begin{aligned} \kappa_3 &= \mathbf{U}^\dagger \mathbf{f}_{\mathbf{R}} \mathbf{R}_3, \\ \lambda_2 &= \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_2 + \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}_2^{(2)}, \\ \nu_0 &= \frac{1}{6} \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uuu}} \mathbf{U} \mathbf{U} \mathbf{U} + \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}_2^{(0)}. \end{aligned} \quad (19)$$

Equation (18) presents a parametric unfolding of dynamics in the vicinity of a *cusplike* bifurcation. Three equilibria — two stable and one unstable — exist in the cusped region

$$\lambda_2 > 0, \quad |\kappa_3| < \frac{2\lambda^{3/2}}{3^{3/2}\nu^{1/2}}. \quad (20)$$

Outside this region, there is a unique stable equilibrium. A *second-order* phase transition occurs when the parameters change in such a way that λ_2 crosses zero. Other transitions occurring in the vicinity of the cusp bifurcation are *weakly* first-order.

The condition $\nu_0 = 0$ defines a singular bifurcation manifold of codimension three. Again, it is possible to fix parametric deviations to suppress the dynamics on the scale t_2 , and obtain in the next order a quartic equation that represents the unfolding of the *butterfly* singularity. The procedure can be continued further if a sufficient number of free parameters is available. The unfolding of a codimension q singularity is presented by a polynomial of order $q + 1$:

$$\partial_q a = \sum_{p=0}^{q-1} \sigma_{q-p+1} a^p + \sigma_0 a^{q+1}, \quad (21)$$

where the parameters σ_k depend on parametric deviations proportional to ε^k .

2.3. Hopf bifurcation

At the Hopf bifurcation point the parametric dependence of the stationary solution $\mathbf{u} = \mathbf{u}_0(\mathbf{R})$ remains smooth; a linear correction can be obtained

from the stationary equation (7), and higher corrections from higher orders of the regular expansion (4). In order to simplify derivations, we shall eliminate this trivial parametric dependence by transforming to a new variable $\hat{\mathbf{u}} = \mathbf{u} - \mathbf{u}_0(\mathbf{R})$. The resulting dynamic system, $d\hat{\mathbf{u}}/dt = \hat{\mathbf{f}}(\hat{\mathbf{u}}, \mathbf{R})$ has the same form as (1) but contains a modified vector-function $\hat{\mathbf{f}}(\hat{\mathbf{u}}, \mathbf{R}) = \mathbf{f}(\hat{\mathbf{u}} + \mathbf{u}_0, \mathbf{R})$. Since, by definition, \mathbf{u}_0 satisfies $\mathbf{f}(\mathbf{u}_0, \mathbf{R}) = 0$, $\hat{\mathbf{u}} = 0$ is a zero of $\hat{\mathbf{f}}(\hat{\mathbf{u}}, \mathbf{R})$. Now we can drop the hats over the symbols and revert to the original form (1) while keeping in mind that $\mathbf{u} = 0$ is a stationary solution for all \mathbf{R} and, consequently, all derivatives $\mathbf{f}_{\mathbf{R}}$, $\mathbf{f}_{\mathbf{R}\mathbf{R}}$, etc. computed at $\mathbf{u} = 0$ vanish.

At a Hopf bifurcation point the Jacobi matrix $\mathbf{f}_{\mathbf{u}}$ has a pair of imaginary eigenvalues $\lambda = \pm i\omega_0$. The first-order Eq. (6) has a nontrivial oscillatory solution

$$\mathbf{u}_1 = a(t_1, t_2, \dots)\Phi(t_0) + c.c.; \quad \Phi(t_0) = e^{i\omega_0 t_0} \mathbf{U} \quad (22)$$

with an arbitrary *complex* amplitude $a(t_1, t_2, \dots)$ dependent on slower time scales t_k , $k > 0$; \mathbf{U} is the eigenvector of $\mathbf{f}_{\mathbf{u}}$ with the eigenvalue $i\omega_0$:

$$\mathbf{f}_{\mathbf{u}}\mathbf{U} = i\omega_0\mathbf{U}. \quad (23)$$

The function $\Phi(t_0)$ and its complex conjugate $\Phi^*(t_0)$ are two eigenfunctions of the linear operator \mathcal{L} , Eq. (6), with zero eigenvalue. The operator \mathcal{L} acts here in the space of $2\pi/\omega_0$ -periodic complex-valued vector-functions with the scalar product defined as

$$\langle \mathbf{u}, \mathbf{v} \rangle = \frac{\omega_0}{2\pi} \int_0^{2\pi/\omega_0} \mathbf{u}^*(t) \cdot \mathbf{v}(t) dt. \quad (24)$$

The eigenfunctions of the adjoint operator $\mathcal{L}^\dagger = \mathbf{f}_{\mathbf{u}}^\dagger + \partial/\partial t_0$ are

$$\Phi^\dagger(t_0) = e^{-i\omega_0 t_0} \mathbf{U}^\dagger$$

and its complex conjugate; \mathbf{U}^\dagger is the eigenvector of $\mathbf{f}_{\mathbf{u}}^\dagger$ with the eigenvalue $i\omega_0$.

The second-order equation can be written in the form

$$\mathcal{L}\mathbf{u}_2 = \partial_1 \mathbf{u}_1 - \frac{1}{2} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{u}_1 \mathbf{u}_1 - \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{u}_1 \mathbf{R}_1. \quad (25)$$

The inhomogeneity of this equation contains both the principal harmonic, $e^{i\omega_0 t_0}$, contributed by the linear terms $\partial_1 \mathbf{u}_1$ and $\mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{u}_1 \mathbf{R}_1$, and terms with

zero and double frequency stemming from the quadratic term $1/2 \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{u}_1 \mathbf{u}_1$. The scalar products of the latter terms with the eigenfunctions $\Phi^\dagger(t_0)$, $\Phi^{\dagger*}(t_0)$ vanish, and the solvability condition of Eq. (25) is obtained in the form:

$$\partial_1 a = \lambda_1 a, \quad (26)$$

where λ_1 is given by Eq. (12) (note that this parameter is now complex).

Equation (26) has a nontrivial stationary solution only if the real part of λ_1 vanishes. This condition defines a hyperplane in the parametric space tangential to the Hopf bifurcation manifold. The imaginary part of λ_1 gives a frequency shift along the bifurcation manifold. In order to eliminate the tangential shift, we set as before $\mathbf{R}_1 = 0$. Then Eq. (26) reduces to $\partial_1 a = 0$, so that the amplitude may evolve only on a still slower scale t_2 . The second-order function \mathbf{u}_2 has to be found by solving Eq. (25), now reduced to the form

$$\mathcal{L}\mathbf{u}_2 = -\frac{1}{2} (a^2 e^{2i\omega_0 t_0} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U} + |a|^2 \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U}^* + c.c.). \quad (27)$$

The solution of this equation is

$$\mathbf{u}_2 = -\frac{1}{2} [|a|^2 \mathbf{f}_{\mathbf{u}}^{-1} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U}^* + a^2 e^{2i\omega_0 t_0} (\mathbf{f}_{\mathbf{u}} - 2i\omega_0)^{-1} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U} + c.c.]. \quad (28)$$

In the third-order,

$$\begin{aligned} \mathcal{L}\mathbf{u}_3 = & \partial_2 \mathbf{u}_1 - \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{u}_1 \mathbf{R}_2 \\ & - \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{u}_1 \mathbf{u}_2 - \frac{1}{6} \mathbf{f}_{\mathbf{u}\mathbf{u}\mathbf{u}} \mathbf{u}_1 \mathbf{u}_1 \mathbf{u}_1. \end{aligned} \quad (29)$$

The amplitude equation is obtained as the solvability condition of this equation. Only the part of the inhomogeneity containing the principal harmonic contributes to the solvability condition, which takes the form

$$\partial_2 a = \lambda_2 a + \nu_0 |a|^2 a, \quad (30)$$

where λ_2 , ν_0 are defined as

$$\begin{aligned} \lambda_2 = & \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{U} \mathbf{R}_2, \\ \nu_0 = & \frac{1}{2} \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U}\mathbf{U}^* - \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} (\mathbf{f}_{\mathbf{u}}^{-1} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U}^*) \\ & - \frac{1}{2} \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}^* ((\mathbf{f}_{\mathbf{u}} - 2i\omega_0)^{-1} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U}\mathbf{U}). \end{aligned} \quad (31)$$

The expansion has to be continued to higher orders, after readjusting the scaling of parametric deviations, if the real part of ν_0 vanishes.

2.4. Automated generation of normal forms

The procedure of derivation of a sequence of amplitude equations described in the preceding section is implemented by the function `BifurcationTheory`.

`BifurcationTheory[operatoreqn, u, R, t, {U, U†}, amp, coef, eps, order, freq, options]` derives a set of amplitude equations for a dynamical system of ordinary differential equations written in an operator form.

`BifurcationTheory` has the following arguments:

- `operatoreqn` denotes an operator equation describing the problem;
- `u` denotes a array of variables;
- `R` denotes a array of bifurcation parameters;
- `t` denotes a time variable;
- `U` and `U†` stand for the normal mode eigenvectors;
- `amp` is an amplitude of the normal mode appearing in the linear solution;
- `coef` denotes the name of coefficients of the resulting amplitude equations;
- `eps` denotes the small parameter of the problem (ε);
- `order` is the highest order of the expansion; if it is higher than the codimension of the bifurcation manifold, corrections to the principal (lowest order) amplitude equation are produced;
- `freq` denotes the frequency of the arising limit cycle (for monotonic bifurcations it can be dropped).

The differentiation operator $\partial/\partial t$ used in the operator equation `operatoreqn` is represented by the symbols `Nabla[t]`. Action of this operator on functional expressions is denoted by the symbol `**` — alias to `NonCommutativeMultiply`.

The function `BifurcationTheory` admits the option `ScalarProduct` specifying a pure function for scalar product used in solvability condition. The default value is `ScalarProduct -> Dot`.

As it is discussed in the preceding section the function automatically shifts the basic solution in the process of derivation of the normal forms for Hopf bifurcation. As for monotonic bifurcations there is no shift with only one exception. In case of

transcritical monotonic bifurcation, where the basic state solution remains constant at all values of parameter, the shift of the solution is admissible. This case needs an application of another option `Transcritical -> True` which forces the function to make a shift in monotonic case. The default value of this option is `Transcritical -> False`.

As an example of usage of the function `BifurcationTheory`, we consider the Hopf bifurcation. Unfortunately, the version 2.2.2 of *Mathematica* used in development of the package has no perfect typesetting abilities of the version 3.0. As a result the output of the function is very lengthy and is difficult to understand for inexperienced users. We present the *Mathematica* output only once and further we will use the standard textbook notation.

The original dynamical problem in the standard notation has a form:

$$\mathbf{u}_t = \mathbf{f}(\mathbf{u}, \mathbf{R}). \quad (32)$$

Hence the first argument `operatoreqn` will take a form: `f[u, R] - Nabla[t]**u == 0` and the function `BifurcationTheory` is used as follows:

```
dynosc bif = BifurcationTheory[
f[u, R] - Nabla[t]**u == 0, u, R, t, {U,
Ut}, a, c, eps, 2, w].
```

The result produced by the function can be presented as a set of two amplitude equations describing the slow dynamics of the amplitude a at the time scales $t_i = \varepsilon^i t_0$, ($i = 1, 2$) [cf. Eqs. (26) and (30)]:

$$\begin{aligned} \{ & \mathbf{a}^{(1,0)}[t[1], t[2]] == \mathbf{a}[t[1], t[2]] \mathbf{c}[2, \\ & 2][R[1]] / \mathbf{c}[2, 1], \\ & \mathbf{a}^{(0,1)}[t[1], t[2]] == \\ & \mathbf{a}[t[1], t[2]]^2 \text{Conjugate}[\mathbf{a}[t[1], t[2]]] \\ & \mathbf{c}[3, 2] / \mathbf{c}[3, 1] + \\ & \mathbf{a}[t[1], t[2]] \mathbf{c}[3, 3][R[1], R[2]] / \mathbf{c}[3, \\ & 1] \}, \end{aligned}$$

or in the usual notation:

$$\begin{aligned} \partial_1 a &= \frac{c_{2,2}(\mathbf{R}_1)}{c_{2,1}} a, \\ \partial_2 a &= \frac{c_{3,2}}{c_{3,1}} |a|^2 a + \frac{c_{3,3}(\mathbf{R}_1, \mathbf{R}_2)}{c_{3,1}} a. \end{aligned} \quad (33)$$

The coefficients c_{ij} of the amplitude equations are generated separately and, hence, can be calculated and simplified separately. The coefficients $c_{2,1} = c_{3,1} = \mathbf{U}\mathbf{U}^\dagger$ determine the normalization of the eigenvectors.

The coefficient in Eq. (26) $\lambda_1 = c_{2,2}(\mathbf{R}_1)/c_{2,1}$. Formulae for calculation of coefficients c are given by the set of the replacement rules:

$$\{c[2, 1] \rightarrow \mathbf{U}^\dagger \cdot \mathbf{U}, \\ c[2, 2][\mathbf{R}[1]] \rightarrow \mathbf{U}^\dagger \cdot \mathbf{f}^{(1,1)}[\mathbf{u}, \mathbf{R}] \cdot \mathbf{U} \cdot \mathbf{R}[1]\}.$$

The second equation is a well-known Landau equation, and the coefficient at the nonlinear term $\nu_0 = c_{3,2}/c_{3,1}$ is called the *Landau coefficient*. The sign of this coefficient determines the type of the bifurcation — the *subcritical* one with unstable limit cycle coefficient arises if the real part of the coefficient is positive, and the *supercritical* otherwise. The unnormalized Landau coefficient $c_{3,2}$ is produced by the function in the following form:

$$c[3, 2] \rightarrow -\mathbf{U}^\dagger \cdot \mathbf{f}^{(2,0)}[\mathbf{u}, \mathbf{R}] \cdot \mathbf{U} \cdot \\ \text{LinearSolve}[\mathbf{f}^{(1,0)}[\mathbf{u}, \mathbf{R}], \mathbf{f}^{(2,0)}[\mathbf{u}, \mathbf{R}]] \cdot \\ \text{DiracConjugate}[\mathbf{U}] \cdot \mathbf{U} - \\ \mathbf{U}^\dagger \cdot \mathbf{f}^{(2,0)}[\mathbf{u}, \mathbf{R}] \cdot \text{DiracConjugate}[\mathbf{U}] \cdot \\ \text{LinearSolve}[-2 \mathbf{I} \text{ w IdentityTensor}[2] + \\ \mathbf{f}^{(1,0)}[\mathbf{u}, \mathbf{R}], \\ \mathbf{f}^{(2,0)}[\mathbf{u}, \mathbf{R}] \cdot \mathbf{U} \cdot \mathbf{U}] / 2 + \\ \mathbf{U}^\dagger \cdot \mathbf{f}^{(3,0)}[\mathbf{u}, \mathbf{R}] \cdot \text{DiracConjugate}[\mathbf{U}] \cdot \mathbf{U} \cdot \\ \mathbf{U} / 2,$$

and can be written in the standard notation as:

$$c_{3,2} = -\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uu}} \mathbf{U} \tilde{\mathbf{U}} \\ - \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \mathcal{R}(-2i\omega \mathbf{I} + \mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U} / 2 \\ - \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uuu}} \mathbf{U} \mathbf{U} \tilde{\mathbf{U}} / 2, \quad (34)$$

where \mathbf{I} denotes the identity matrix, which corresponds to the `IdentityTensor[2]` (tensor of the rank 2) generated by the function `BifurcationTheory`. The $\mathcal{R}(\mathbf{m})$ denotes the resolvent matrix of the matrix \mathbf{m} — if the matrix is regular, resolvent coincides with the inverse matrix, otherwise, resolvent is constructed using the spectrum of the original matrix \mathbf{m} . A special function `Resolvent[matrix]` is designed for the construction of the resolvent of a singular matrix.

Finally the linear term coefficient in the Landau equation depends on parametric deviations of the first- and second-order:

$$c_{3,3}(\mathbf{R}_1, \mathbf{R}_2) \\ = (\mathbf{U}^\dagger \mathcal{R}(-i\omega \mathbf{I} + \mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_1) (\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_1) / (\mathbf{U}^\dagger \mathbf{U}) \\ + \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_2 - \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathcal{R}(-i\omega \mathbf{I} + \mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_1 \mathbf{R}_1 \\ + \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uRR}} \mathbf{U} \mathbf{R}_1 \mathbf{R}_1 / 2. \quad (35)$$

It can be easily seen that the condition $\mathbf{R}_1 = 0$ reduces the above general expression to linear coefficient λ_2 in (31) depending on \mathbf{R}_2 only.

The case of a monotonic bifurcation is more complicated, the resulting formulae are more cumbersome, and we present the results of the *Mathematica* calculations in the standard notation. It must be noted that it has been indicated in the previous section that the first-order parametric deviation \mathbf{R}_1 is automatically set to zero.

The set of two amplitude equations describing the slow dynamics of the amplitude a now takes a form:

$$\partial_1 a = \frac{c_{2,2}}{c_{2,1}} a^2 + \frac{c_{2,3}(\mathbf{R}_2)}{c_{2,1}}, \quad (36) \\ \partial_2 a = \frac{c_{3,2}}{c_{3,1}} a^3 + \frac{c_{3,3}(\mathbf{R}_2)}{c_{3,1}} a + \frac{c_{3,4}(\mathbf{R}_3)}{c_{3,1}}.$$

Now the nontrivial amplitude equation appears already at the first time scale t_1 . It contains quadratic in amplitude term with unnormalized coefficient given by:

$$c_{2,2} = \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U} / 2, \quad (37)$$

and corresponds to μ_0 in (12); the coefficient $c_{2,3}$ coincides with κ_2 in (12).

The equation at the slower time scale gives corrections to the principal equation. Its Landau coefficient can be cast as follows:

$$c_{3,2} = (\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}) (\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}) / (2 \mathbf{U}^\dagger \mathbf{U}) \\ - \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U} / 2 \\ + \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uuu}} \mathbf{U} \mathbf{U} \mathbf{U} / 6. \quad (38)$$

The linear term coefficient is given as:

$$c_{3,3}(\mathbf{R}_2) \\ = \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_2 \\ + (\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U}) (\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_2) / (\mathbf{U}^\dagger \mathbf{U}) \\ - \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{R}} \mathbf{R}_2. \quad (39)$$

Finally the free term in the equation coincides with κ_3 in (19).

2.5. Computation of coefficients

2.5.1. Function CalculateCoefficient

In order to perform the calculation of the coefficient of the amplitude equations describing slow dynamics in the vicinity of a bifurcation point of a particular problem it is needed to specify values of all elements in the output of the function `BifurcationTheory`, substitute them into the formulae and carry out required simplifications. The last two steps of this procedure is performed automatically by the function `CalculateCoefficient`.

`CalculateCoefficient[coefrule, urule, Rrule, freqrule, funcrules, eigenrules, addrules]` performs calculation of the rule for the coefficient of the amplitude equations provided by the function `BifurcationTheory` using the rules specifying the required data.

`CalculateCoefficient` has the following arguments:

- `coefrule` denotes a rule for the coefficient of the amplitude equations produced by the function `BifurcationTheory`;
- `urule` specifies the names of the state vector components with their critical values at the bifurcation point;
- `Rrule` specifies the names of the bifurcation parameter vector components with their critical values at the bifurcation point;
- `freqrule` specifies the values, wavenumber and frequency at the bifurcation point;
- `funcrules` denotes an array of rules specifying all functional and constant objects (array, matrices, tensors, etc.) appearing in the output of the function `BifurcationTheory`;
- `eigenrules` denotes an array of rules specifying values of the eigenvectors of the problem;
- `addrules` denotes an array of additional rules needed for calculations (for example, restrictions on the parametric deviations); this argument can be dropped.

The function `CalculateCoefficient` has the only option `ComplexTheory` specifying the names of the state vector components assumed to be complex-valued. The default value of the option is `ComplexTheory -> None`. Example of the usage is presented in Appendix A.

2.5.2. Lorenz model

The well-known Lorenz system [Lorenz, 1963], that has been originally suggested as a qualitative model

of cellular convection, exhibits rich dynamic behavior including periodic and chaotic motion. It also possesses a monotonic bifurcation that corresponds to a primary transition from the quiescent state to convection. In usual notation, the Lorenz system is written as

$$\begin{aligned} dx/dt &= -\sigma(x - y), \\ dy/dt &= x(R - z) - y, \\ dz/dt &= -bz + xy. \end{aligned}$$

The linear analysis made with *Mathematica* which is presented in the Appendix A locates the bifurcation point at $x = y = z = 0$ and $R = 1$; the eigenvectors are $\mathbf{U} = \{1, 1, 0\}$ and $\mathbf{U}^\dagger = \{1/\sigma, 1, 0\}$. Calculations of the coefficients performed in Appendix A shows that the lowest-order equation is trivial $-\partial_1 a = 0$. The Landau equation has the form:

$$\partial_2 a = \frac{\sigma}{1 + \sigma}(-a^3/b + aR_2).$$

The result proves that the bifurcation is always supercritical at physical (positive) values of the parameters.

2.5.3. Brusselator model

The next example is a well-known Brusselator model of chemical oscillations [Nicolis & Prigogine, 1977]:

$$\begin{aligned} dz/dt &= a - (1 + b)z + uz^2, \\ du/dt &= bz - uz^2. \end{aligned}$$

The real variables u, z denote concentrations of the “activator” and “inhibitor” species. The unique stationary solution $z = a, u = b/a$ bifurcates into the limit cycle at $b = 1 + a^2$. Calculations can be made only after elimination of the parametric dependence of the basic solution made by the shifting of the basic solution to zero. The shifted system has the following form:

$$\begin{aligned} dz/dt &= a^2 u - z + bz + 2auz + bz^2/a + uz^2, \\ du/dt &= -a^2 u - bz - 2auz - bz^2/a - uz^2. \end{aligned}$$

The linear analysis of the problem is presented in Appendix B. The eigenvectors at the Hopf bifurcation point are $\mathbf{U} = \{a/(i - a), 1\}$ and $\mathbf{U}^\dagger = \{(i + a)/a, 1\}$.

The calculation produces the following results for the coefficients in the first equation from (33):

$$\begin{aligned} c_{2,1} &= \frac{2}{1+ia}; \\ c_{2,2}(\mathbf{R}_1) &= \frac{b_1}{1+ia}. \end{aligned} \quad (40)$$

Setting $b_1 = 0$ one can proceed to the next order:

$$\begin{aligned} c_{3,1} &= \frac{2}{1+ia}; \\ c_{3,2} &= \frac{4-6ia-7a^2-3ia^3+4a^4}{3ia(1+a^2)(1+ia)}; \\ c_{3,3}(\mathbf{R}_1, \mathbf{R}_2) &= \frac{b_2}{1+ia}. \end{aligned} \quad (41)$$

The Landau coefficient at the nonlinear term finally takes a form

$$\frac{4-6ia-7a^2-3ia^3+4a^4}{6ia(1+a^2)};$$

it is easy to see that its real part simplifies to $-(1+1/2a^2)/(1+a^2)$, and is negative definite, hence, the bifurcation is always supercritical.

2.5.4. Exothermic reaction in a stirred tank reactor

The following example involves somewhat heavier computations, and necessitates the use of implicit functions. Consider a dynamical system describing an exothermic reaction in a continuous stirred tank reactor [Uppal *et al.*, 1974; Pismen, 1986]:

$$\begin{aligned} dx/dt &= (1-x)e^y - mx, \\ g dy/dt &= h(1-x)e^y - my. \end{aligned} \quad (42)$$

The variables x , y denote the conversion and dimensionless temperature, respectively; h is the exothermicity parameter, m is the dimensionless flow rate, and g is the thermal capacitance factor that equals to unity in an adiabatic reactor and decreases with intensified cooling. This model exhibits both monotonic and Hopf bifurcations. Equilibria of Eq. (42) do not depend on the parameter g , so conditions of a monotonic bifurcation can depend on two independent parameters m , h only; the maximal codimension is two (a cusp point).

Monotonic bifurcation. Consider first a bifurcation manifold of codimension one (a fold line)

for a simplified model with $g = 1$. We localize this bifurcation as before — the bifurcation locus parametrized by the stationary value y_s of the variable y can be found with the help of the standard *Mathematica* function `Solve`. This parametrization is advantageous, since if one of the actual parameters h or m was used, either two or no solutions were obtained in different parametric domains, and the form of the solution was more complicated. The manifold is given as:

$$x = 1 - \frac{1}{y_s}, \quad m = \frac{e^{y_s}}{y_s - 1}, \quad h = \frac{y_s^2}{y_s - 1}.$$

The admissible values of y_s are restricted by the condition $y_s > 1$. The eigenvectors of the problem can be written as $\mathbf{U} = \{(-1+y_s)/y_s^2, 1\}$ and $\mathbf{U}^\dagger = \{-y_s, 1\}$. The calculation process is similar to that of the preceding subsections with only exception — the bifurcation parameters vector now has two components h and m . The lowest-order amplitude equation takes a form:

$$\partial_1 a = \frac{e^{y_s}(2-y_s)}{2(y_s-1)}a^2 + e^{y_s}h_2 - y_sm_2. \quad (43)$$

One can proceed further in order to find corrections (parametric deviations of the third-order are set to zero):

$$\begin{aligned} \partial_2 a &= \frac{e^{y_s}(3-2y_s)}{6(y_s-1)}a^3 \\ &+ \left(\frac{e^{y_s}(2-2y_s+y_s^2)}{2y_s^2}h_2 - m_2 \right)a. \end{aligned} \quad (44)$$

Cusp point. The loci of fold bifurcation in the parametric plane h , m , drawn as a parametric plot, are shown in Fig. 1. The two branches join with a common tangent at the cusp point. In the vicinity of this point, the applicable amplitude equation will include a restriction on deviations of both parameters that specify the direction of this common tangent. It can be easily seen that the quadratic term in the lowest-order Eq. (43) vanishes at $y_s = 2$ where the cusp point is located. The equation becomes trivial at $h_2 = 2m_2/e^2$. This relation defines a direction in the parametric space along which the second-order deviation is made. The next order deviation must be orthogonal to this direction. In the

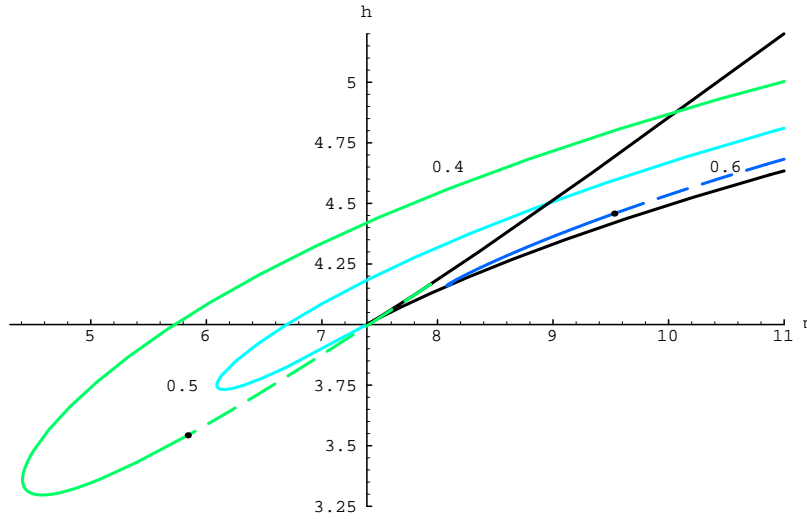


Fig. 1. Loci of fold and Hopf bifurcation in the parametric plane h, m . The three Hopf curves correspond to $g = 0.4, 0.5$ and 0.6 . Solid gray lines show the supercritical, and dashed lines, the subcritical bifurcation. Outside the cusped region, the unique stationary state suffers oscillatory instability within the loop of the Hopf bifurcation locus. Within the cusped region, there are three stationary states, of which two, lying on the upper and lower folds of the solution manifold, may be stable. The solutions on the upper fold are unstable below the Hopf bifurcation line.

vicinity of this point the Landau equation is cast into (m_3 is set to zero):

$$\partial_2 a = -\frac{e^2}{6} a^3 + m_2 a + e^2 h_3. \tag{45}$$

Hopf bifurcation. The dynamical system (42) can also undergo a Hopf bifurcation. In the operator form it can be written as:

$$\mathbf{G}(\mathbf{R})\mathbf{u}_t = \mathbf{f}(\mathbf{u}), \tag{46}$$

where $\mathbf{G}(\mathbf{R})$ denotes a capacitance matrix.

The function `BifurcationTheory` called for this type of the problem produces the set (33) of the amplitude equations (at the Hopf bifurcation point) with the following formulae for the coefficients of the first amplitude equation:

$$\begin{aligned} c_{2,1} &= \mathbf{U}^\dagger \mathbf{G} \mathbf{U}; \\ c_{2,2}(\mathbf{R}_1) &= -i\omega \mathbf{U}^\dagger \mathbf{G}_R \mathbf{U} \mathbf{R}_1. \end{aligned} \tag{47}$$

The Landau coefficient in the second equation is given by (35) with the only replacement of the identity matrix \mathbf{I} by the capacitance matrix \mathbf{G} . Expression for the coefficient $c_{3,3}(\mathbf{R}_1, \mathbf{R}_2)$ of the linear term is not shown due to its complexity.

We start the computations from the determination of the Hopf bifurcation manifold. It contains

stationary points of the system at which a matrix $\mathbf{f}_u - i\omega \mathbf{G}$ is singular (ω denotes the frequency of the limit cycle). The manifold is given by the following set of equations:

$$\begin{aligned} e^y(h - y) - my &= 0, \\ e^y(g + y - h) + m(1 + g) &= 0. \end{aligned}$$

These equations are solved to express the values of the parameters m and h through the stationary value $y = y_0$ and the remaining parameter $g = g_0$; y_0, g_0 are thus chosen to parameterize the 2D Hopf bifurcation manifold in the 3D parametric space:

$$\begin{aligned} h &= y_0 + \frac{g_0 y_0}{y_0 - g_0 - 1}, \\ m &= \frac{g_0 e^{y_0}}{y_0 - g_0 - 1}. \end{aligned}$$

The loci of Hopf bifurcation in the parametric plane h, m at several chosen values of g are shown in Fig. 1. Outside the cusped region, the unique stationary state suffers oscillatory instability within the loop of the Hopf curve (this is possible at $g < 1/2$ only). Within the cusped region, the solutions on the upper fold are unstable below the Hopf bifurcation line. The solutions at the lower fold can also suffer oscillatory instability at lower values of g .

Now it is possible to compute the frequency $w = e^{y_0} \sqrt{y_0 - g_0 y_0 - 1} / (1 + g_0 - y_0)$ and the eigenvectors:

$$\mathbf{U} = \left\{ \frac{g(1 - y_0 - i\sqrt{y_0 - g_0 y_0 - 1})}{y_0(y_0 - 1)}, 1 \right\};$$

$$\mathbf{U}^\dagger = \left\{ (y_0 - 1) \frac{g_0(1 - y_0 + i\sqrt{y_0 - g_0 y_0 - 1})}{1 + g_0 - y_0}, 1 \right\}.$$

(48)

As it was done above, one can choose the parametric deviation of the first-order in such a way as to make the first amplitude equation trivial. Then the Landau coefficient in the second equation can be presented after normalization as:

$$c_{3,2}/c_{3,1} = (y_0 - g_0 y_0 - 1)^{3/2} (i y_0 - i - \sqrt{y_0 - g_0 y_0 - 1})^{-1} e^{y_0} / 12$$

$$\times (12 - 24g_0 - 24y_0 + 40g_0 y_0 - 4g_0^2 y_0 + 14y_0^2 - 21g_0 y_0^2 + 4g_0^2 y_0^2 - 2y_0^3 + 2g_0 y_0^3 + i\sqrt{y_0 - g_0 y_0 - 1}(-12 + 24g_0 + 15y_0 - 25g_0 y_0 - 2g_0^2 y_0 - 5y_0^2 + 8g_0 y_0^2)).$$

(49)

First, we take note that only a part of the parametric plane y_0, g_0 above the thick solid curve in Fig. 2 is actually available, since the condition of positive oscillation frequency requires

$$y_0 - g_0 y_0 - 1 > 0. \tag{50}$$

Within this region, the limit cycle is stable (the bifurcation is *supercritical*) if the real part of the coefficient at the nonlinear term is negative. Extracting the real part from (49) brings this condition to the form

$$\frac{3g_0 + 2g_0^2 + 2y_0 - 4g_0 y_0 - 2g_0^2 y_0 - y_0^2 + 2g_0 y_0^2 - 1}{4(y_0 - 1 - g_0)(y_0 - g_0 y_0 - 1)} < 0. \tag{51}$$

Noting that the denominator of the above fraction is positive whenever the inequality (50) is verified, one can determine the stability boundary by equating the numerator in (51) to zero, and combining the result with (50). The stability boundary in the plane (g_0, y_0) , separating the regions of subcritical and supercritical bifurcation is shown in Fig. 2;

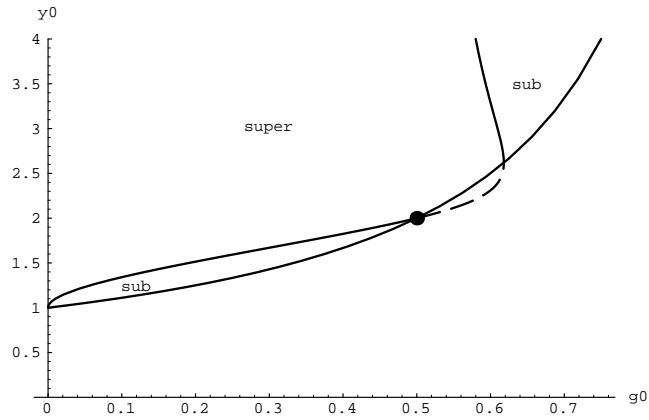


Fig. 2. The stability boundary in the plane (g_0, y_0) , separating the regions of subcritical and supercritical Hopf bifurcation. The unphysical part of the curve below the boundary of positive frequency is shown by a dashed line. The solid circle at $g_0 = 0.5, y_0 = 2$ marks the double zero point.

the unphysical part of the curve dipping below the boundary of positive frequency is shown by a dashed line. The region of subcritical bifurcations consists of two disconnected parts, of which the lower one lies within the region of unique stationary states and on the lower fold of the solution manifold, and the upper one, on the upper fold in the region of multiple solutions.

3. General Algorithm for Distributed Systems

3.1. Introduction

The main point of our approach can be formulated as follows. An algorithm applicable to the nonlinear analysis of a number of representative realistic problems must be as general as possible, i.e. it must be designed for classes of problems (say, dynamical problems, or reaction–diffusion type problems), or even better, it should embrace *all* problems which can be solved using standard methods of bifurcation expansion.

It is clear that the generalization from particular problems to some class of such problems can be performed using an operator form of the problem. For example, all reaction–diffusion type problems can be presented in the following operator form:

$$\mathbf{G}(\mathbf{R}) \frac{\partial}{\partial t} \mathbf{u}(\mathbf{r}, t) = \mathbf{D}(\mathbf{R})(\nabla \cdot \nabla) \mathbf{u}(\mathbf{r}, t) + \mathbf{f}(\mathbf{u}(\mathbf{r}, t), \mathbf{R}), \tag{52}$$

where $\partial/\partial t$ denotes the time differentiation operator, ∇ stands for the operator of differentiation over the spatial variable \mathbf{r} ; $\mathbf{f}, \mathbf{u}, \mathbf{R}$ are arrays of functions, variables and bifurcation parameters of the problem. $\mathbf{G}(\mathbf{R})$ and $\mathbf{D}(\mathbf{R})$ denote capacitance and diffusion matrix respectively, which can depend on the bifurcation parameters.

In its turn problem (52) appears to be a particular case of most general problem which can be written as

$$\mathbf{F}(\nabla, \partial/\partial t, \mathbf{u}(\mathbf{r}, t, \mathbf{R}), \mathbf{R}) = 0, \quad (53)$$

where \mathbf{F} can also include a set of boundary conditions imposed on the solution $\mathbf{u}(\mathbf{r}, t, \mathbf{R})$.

3.2. Linear analysis and dispersion relation

The general standard algorithm for derivation of amplitude equations starts from the linear analysis of an underlying distributed system in the vicinity of a basic state. We assume also that for each value \mathbf{R} the system admits a stationary spatially homogeneous solution $\mathbf{u}_0(\mathbf{R})$, which is called *basic state*. Typically the basic state becomes unstable in a certain domain of the parametric space, and this instability is usually connected with the bifurcations of new solutions with a more complicated spatiotemporal structure. We construct solutions of the original problem (53) in the form $\mathbf{u} = \mathbf{u}_0(\mathbf{R}) + \tilde{\mathbf{u}}(\mathbf{r}, t, \mathbf{R})$, where $\tilde{\mathbf{u}}$ is a *small disturbance* of the basic state. Substituting the solution in (53) one arrives in the linear approximation in $\tilde{\mathbf{u}}$ to the following:

$$\mathcal{L}(\nabla, \partial/\partial t, \mathbf{u}_0(\mathbf{R}), \mathbf{R})\tilde{\mathbf{u}} = 0, \quad (54)$$

where \mathcal{L} is a linear operator (Frechet derivative) calculated at the point $\mathbf{u} = \mathbf{u}_0$ acting on small disturbance $\tilde{\mathbf{u}}$. Further on, we shall consider *normal disturbances* of the form:

$$\tilde{\mathbf{u}}(\mathbf{r}, t, \mathbf{R}) = \mathbf{A}(\mathbf{k}, \mathbf{R}) \exp(\sigma t + i\mathbf{k}\mathbf{r}). \quad (55)$$

The growth rate σ is generally a complex number. For normal disturbances the evolution equation (54) is reduced to the eigenvalue problem:

$$\mathcal{L}(i\mathbf{k}, \sigma, \mathbf{u}_0(\mathbf{R}), \mathbf{R})\mathbf{A} = 0, \quad (56)$$

which usually determines a countable set of branches of *dispersion relation* between growth rates σ_n and the wavenumber $k = |\mathbf{k}|$. We assume

that the instability is generated by eigenmodes with the growth rates $\sigma_j(k, \mathbf{R}) = \sigma_{jr}(k, \mathbf{R}) + i\omega_j(k, \mathbf{R})$. The conditions $\sigma_{jr}(k, \mathbf{R}) = 0$ determine instability boundaries which are called *neutral stability curves*. The minima of all functions $\sigma_{jr}(k, \mathbf{R})$ are reached at the same value $\mathbf{R} = \mathbf{R}_0$ and at (possibly various) values $k = k_{jc}$.

If $\omega_j(k_{jc}, \mathbf{R}_0) = 0$, the corresponding instability is called *stationary* (monotonous); otherwise, there is an *oscillatory* (wavy) instability. In each of these cases, two possibilities arise depending on the wavenumber critical value: Either the instability arises near a *nonzero* wavenumber k_{jc} (*short-wavelength* instability), or the instability domain is localized around $k_{jc} = 0$ (*long-wavelength* instability).

The linear analysis procedure also includes determination of eigenvectors $\mathbf{U}_j, \mathbf{U}_j^\dagger$ of the linear problem (56) verifying the equation $\mathcal{L}\mathbf{U}_j = 0$ and its adjoint counterpart $\mathcal{L}^\dagger\mathbf{U}_j^\dagger = 0$ needed for further calculations. Setting aside most complicated cases of double and triple bifurcation points we, however, permit simple degenerate cases, when each instability mode is characterized by a unique set of wavevector and frequency values.

A general solution \mathbf{u}_l of the linear problem (54) can be written as a superposition of several normal modes with j th mode characterized by its scalar amplitude a_j , particular values of the wavevector \mathbf{k}_j , time frequency ω_j , eigenvector of the mode \mathbf{U}_j and its order of smallness d_j :

$$\begin{aligned} \mathbf{u}_l = \varepsilon^{d_0} a_0 \mathbf{U}_0 + \sum_{j=1}^N \varepsilon^{d_j} (a_j \mathbf{U}_j \exp(i\mathbf{k}_j \mathbf{r}_0 + i\omega_j t_0) \\ + a_j^* \tilde{\mathbf{U}}_j \exp(-i\mathbf{k}_j \mathbf{r}_0 - i\omega_j t_0)), \end{aligned} \quad (57)$$

where $*$ denotes an operation of the complex conjugation and $\tilde{}$ denotes an operation of Dirac conjugation, which in the case of real vector function \mathbf{F} is reduced to the standard complex conjugation. The coefficient $a_0 \neq 0$ if monotonic long-scale mode characterized by the zero value of the wavenumber and time frequency is permitted. Each mode gives rise to a corresponding solvability condition which determines a slow spatiotemporal dynamics of the mode's amplitude using the consequent orders of the multiscale expansion of the problem.

3.3. Multiscale expansion

In order to simplify derivations, we shall eliminate trivial parametric dependence of the basic state by

transforming to a new variable $\hat{\mathbf{u}} = \mathbf{u} - \mathbf{u}_0(\mathbf{R})$. The resulting system, $\mathbf{F}(\nabla, \partial/\partial t, \hat{\mathbf{u}} + \mathbf{u}_0, \mathbf{R}) = 0$ has the same form as (53) but contains a modified operator $\hat{\mathbf{F}}(\nabla, \partial/\partial t, \hat{\mathbf{u}}, \mathbf{R}) = \mathbf{F}(\nabla, \partial/\partial t, \hat{\mathbf{u}} + \mathbf{u}_0, \mathbf{R})$. Since, by definition, \mathbf{u}_0 satisfies $\mathbf{F}(\nabla, \partial/\partial t, \mathbf{u}_0, \mathbf{R}) = 0$, $\hat{\mathbf{u}} = 0$ is a zero of $\hat{\mathbf{F}}(\nabla, \partial/\partial t, \hat{\mathbf{u}}, \mathbf{R})$. Now we can drop the hats over the symbols and revert to the original form (53) while keeping in mind that $\mathbf{u} = 0$ is a stationary solution for all \mathbf{R} and, consequently, all derivatives $\mathbf{F}_{\mathbf{R}}, \mathbf{F}_{\mathbf{R}\mathbf{R}}$, etc. computed at $\mathbf{u} = 0$ vanish.

We use the expansions (2) for variables and parameters and introduce a hierarchy of time scales t_k , thus replacing the function \mathbf{u} by a function of an array of rescaled time variables. Accordingly, the time derivative is expanded as in (3). The spatial derivative is expanded similarly:

$$\nabla = \nabla_0 + \varepsilon^\alpha \nabla_1, \tag{58}$$

where α denotes the spatial scaling which depends on a particular problem; for the sake of simplicity, we shall use only positive integer values of α . Substituting expansions (2) and (3) and (58) into the original problem (53) and expanding in ε , one arrives at a set of equations for different orders of ε .

In the lowest-order we reproduce the equation $\mathbf{F}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0) = 0$ determining the basic solution computed at the critical values of bifurcation parameters. In the next order the linear problem (54) is reproduced in the following form:

$$\mathbf{F}_{\mathbf{u}}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0)\mathbf{u}_1 = 0. \tag{59}$$

The solution \mathbf{u}_1 consists of normal modes with $d_j = 1$.

In the consequent orders one arrives at the equations of the form:

$$\mathbf{F}_{\mathbf{u}}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0)\mathbf{u}_n = \mathbf{g}_n, \tag{60}$$

where \mathbf{g}_n denotes the n th order inhomogeneity vector. A set of solvability conditions for each of the normal modes appearing in the linear solution (57) will define slow spatiotemporal dynamics of the amplitude of each mode. It can be shown that only part of the inhomogeneity \mathbf{g}_n which projects on the principal harmonic of a certain mode will contribute to the corresponding solvability condition. Denoting the scalar product by angle brackets and the projection operator on the harmonic $\exp(i\beta)$ as $\mathcal{P}(\cdot, \exp(i\beta))$, one can write the solvability condition for j th normal mode in the n th order as

follows:

$$\langle \mathbf{U}_j^\dagger, \mathcal{P}(\mathbf{g}_n, e^{i\mathbf{k}_j \mathbf{r}_0 + i\omega_j t_0}) \rangle = 0, \tag{61}$$

where \mathbf{U}_j^\dagger denotes the eigenvector of the adjoint linear problem $\mathcal{L}^\dagger \mathbf{U}_j^\dagger = 0$ corresponding to the j th mode.

The linear inhomogeneous problem (60) must be solved with respect to \mathbf{u}_n provided solvability conditions (61) are satisfied. To this particular solution of (60) one must add a linear solution term of the corresponding order of smallness. The combined solution is used for the calculations of the next order inhomogeneity \mathbf{g}_{n+1} .

In the second-order the vector of inhomogeneity \mathbf{g}_2 can be represented in the form:

$$\begin{aligned} \mathbf{g}_2 = & -\frac{1}{2}\mathbf{F}_{\mathbf{u}\mathbf{u}}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0)\mathbf{u}_1\mathbf{u}_1 \\ & - \mathbf{F}_{\mathbf{u}\mathbf{R}}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0)\mathbf{u}_1\mathbf{R}_1 \\ & - \delta_{\alpha,1}\mathbf{F}_{\mathbf{u}\nabla}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0)\nabla_1\mathbf{u}_1 \\ & - \mathbf{F}_{\mathbf{u}\frac{\partial}{\partial t}}(\nabla_0, \partial_0, \mathbf{u}_0, \mathbf{R}_0)\partial_1\mathbf{u}_1, \end{aligned} \tag{62}$$

where the Kronecker symbol $\delta_{\alpha,\beta} = 0$ at $\alpha \neq \beta$ and $\delta_{\alpha,\alpha} = 1$. The resulting set of the conditions in the second-order is resolved further with respect to the derivative of the amplitudes $\partial_1 a_j$. This result presents the set of the amplitude equations of the second-order and in its turn is used for derivation of the amplitude equations in the next orders.

The final result is the set of the amplitude equations written in most general form which is valid for the combination of the normal modes in (57) and specified value of the spatial variable scaling exponent α . This set further can be “projected” onto a particular class of the problems to produce a required formula. These formulae are applicable to any problem from the selected class. In order to make actual calculations for a particular problem one must determine the values of the wavevectors, frequency, eigenvectors, etc. and substitute them into the abovementioned formulae.

3.4. *Function* BifurcationTheory

The function `BifurcationTheory` used for derivation of the normal forms for dynamical systems can be applied with some additions to distributed systems.

If it is required to derive the normal form for a *single* mode arising at a bifurcation point of the distributed system, one may use the call

```
BifurcationTheory[operatoreqn, u, R, t,
{r, dim}, spatscale, {U, U†},
amp, coef, eps, order, wavenumber, freq,
opts].
```

Here \mathbf{r} denotes a spatial variable (that can be a vector); dim is the space dimension and spatscale denotes an array consisting of the name of the spatial variable and its (integer) scaling exponent α . Finally, wavenumber must be set equal to zero for a long-scale instability and to some symbol in the short-scale case. In the latter case the wavevector needed for the calculations is generated automatically. The differentiation operators $\partial/\partial t$ and ∇ used in the operator equation `operatoreqn` are represented by the symbols `Nabla[t]` and `Nabla[r]`, respectively.

A more complicated form must be used in a case when there is an angular degeneracy of the normal modes, namely, when the different modes have the same values of their parameters but the wavevectors with equal lengths have different directions. It is rational to specify the mode data using the angular measurement for the wavevectors —

```
BifurcationTheory[operatoreqn, u, R, t,
{r, dim}, spatscale, {U, U†},
amps, coef, eps, order, wavenumber, freq,
ampout, opts],
```

where `amps` consists of the pairs $\{a_j, \beta_j\}$ with β_j denoting an angle between the wavevector of the j th mode a_j and some selected direction. If the argument `ampout` specifying the names of the amplitudes for which equations must be generated is omitted, equations for first amplitude only from the array `amps` would be produced.

The most general form of the function is used for algebraically degenerated cases:

```
BifurcationTheory[operatoreqn, u, R, t,
{r, dim}, spatscale, amps,
coef, eps, order, ampout, options]
```

derives a set of amplitude equations for a distributed system of partial differential equations written in an operator form. Here `amps` is an array of elements specifying the normal modes appearing in the linear solution (57). Each item of `amps` is an array of six elements in the following order — amplitude of the mode (a_j), mode wavevector (\mathbf{k}_j),

time frequency (ω_j), eigenvector (\mathbf{U}_j), eigenvector of the adjoint problem (\mathbf{U}_j^\dagger), and order of smallness of the normal mode (d_j). `ampout` again denotes an array of the amplitude names for which the amplitude equations must be generated.

4. Amplitude Equations for Reaction–Diffusion Problems

4.1. Long-scale instabilities

In this and the next subsections we present the result of derivation of the amplitude equations for reaction–diffusion problem (52) with capacitance matrix \mathbf{G} equal to identity matrix \mathbf{I} and diffusivity matrix \mathbf{D} which does not depend on the bifurcation parameters.

We start from the case where the instability domain is localized around $k_c = 0$ restricting ourselves to nondegenerated nonresonant cases.

The operator equation corresponding to the problem may be written as:

$$\text{DD} \cdot (\text{Nabla}[\mathbf{r}] \cdot \text{Nabla}[\mathbf{r}]) \mathbf{u} + \mathbf{f}[\mathbf{u}, \mathbf{R}] - \text{Nabla}[\mathbf{t}] \mathbf{u} == 0$$

where `DD` denotes the diffusivity matrix. Operator `Nabla[r]` is assumed to be vectorial, hence the scalar Laplacian is written as scalar product of two differential operators. The function is called as follows:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] -
Nabla[t]**u == 0,
u, R, t, {r,2},{r,1},{U,Ut}, a, c, eps, 2,
0, 0]
```

Unfortunately, the version 2.2.2 of *Mathematica* used in development of the package has no perfect typesetting abilities like the version 3.0. As a result the output of the function is very lengthy and is difficult to understand for the inexperienced user. Here and further, we present output produced by the function `BifurcationTheory` using standard textbook notation.

The result produced by the function coincides with that of the monotonic bifurcation of the dynamical system (36) with the only exception — the Landau equation is converted into the Ginzburg–Landau equation with an additional diffusional term of the form:

$$\frac{\mathbf{U}^\dagger \mathbf{D} \mathbf{U}}{\mathbf{U}^\dagger \mathbf{U}} (\nabla_1 \nabla_1) a. \quad (63)$$

Now we turn to the case of the Hopf bifurcation for the same problem. The last argument of the function `BifurcationTheory` denoting the limit cycle frequency now is set to `w` rather than zero:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] -
Nabla[t]**u == 0,
u, R, t, {r,2},{r,1},{U,Ut}, a, c, eps, 2,
0, w]
```

As in the previous case the resulting set of equations is given by (33) with the addition of the same diffusional term.

4.2. Turing bifurcation

Short-scale instabilities are characterized by a nonzero value of the wavenumber; hence, several modes with different directions of the wavevector are permitted.

This case is characterized by the nonzero value of the wavenumber and zero frequency, what is reflected in the function is called:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] -
Nabla[t]**u == 0,
u, R, t, {r,2},{r,1},{U,Ut},
{{a1,0}, {a2, alpha}}, c, eps, 2, k, 0]
```

It corresponds to the case of two normal modes with a wavenumber equal to k — a wavevector \mathbf{k}_1 of the first mode a_1 is directed along the x -axis in a plane (the dimension of spatial variable is set equal to 2); the wavevector \mathbf{k}_2 of the second mode a_2 makes the angle α with \mathbf{k}_1 . We assume that this angle is not equal to $\pi/3$ or $2\pi/3$ in order to make these two modes nonresonant. The argument specifying names of the amplitudes for output is omitted, so the equations for amplitude a_1 are only generated by default.

The result may be written as:

$$\begin{aligned} \partial_1 a_1 &= \frac{c_{2,1,1}}{c_{2,2}} (i\mathbf{k}_1 \nabla_1) a_1 + \frac{c_{2,3}(\mathbf{R}_1)}{c_{2,2}} a_1, \\ \partial_2 a_1 &= \frac{c_{3,4}}{c_{3,3}} |a_2|^2 a_1 + \frac{c_{3,5}}{c_{3,3}} |a_1|^2 a_1 \\ &+ \frac{c_{3,6}(\mathbf{R}_1, \mathbf{R}_2)}{c_{3,3}} a_1 + \frac{c_{3,1,1}}{c_{3,3}} (\nabla_1 \nabla_1) a_1 \\ &+ \frac{c_{3,1,2}}{c_{3,3}} (i\mathbf{k}_1 \nabla_1)^2 a_1 + \frac{c_{3,2,1}(\mathbf{R}_1)}{c_{3,3}} (i\mathbf{k}_1 \nabla_1) a_1. \end{aligned} \quad (64)$$

The coefficients $c_{2,2} = c_{3,3} = \mathbf{U}^\dagger \mathbf{U}$ determine a normalization of the eigenvectors.

For the first time scale t_1 we have a linear equation. Its linear term coefficient is proportional to the first-order deviation of the bifurcation parameter vector and is given by (26). The differential term has a coefficient of the form

$$c_{2,1,1} = 2\mathbf{U}^\dagger \mathbf{D} \mathbf{U}. \quad (65)$$

Choosing the parametric deviation \mathbf{R}_1 one may set the real part of the linear term coefficient equal to zero; then the resulting equation will admit a traveling wave solution.

The Ginzburg–Landau equation at the slower time scale is most interesting. It contains two nonlinear terms describing interaction between the two modes as well as the self-interaction of the principal mode a_1 . Interaction coefficient $c_{3,4}$ of two modes depends on the angle α between their wavevectors and is calculated using the formula:

$$\begin{aligned} c_{3,4} &= -\mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2k^2 \mathbf{D}(1 - \cos \alpha)) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2k^2 \mathbf{D}(1 + \cos \alpha)) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} \\ &+ \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} \tilde{\mathbf{U}}. \end{aligned} \quad (66)$$

The self-interaction coefficient $c_{3,5}$ may be found as half of the value of $c_{3,4}$ calculated at $\alpha = 0$:

$$\begin{aligned} c_{3,5} &= -\mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 4k^2 \mathbf{D}) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} / 2 \\ &+ \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} \tilde{\mathbf{U}} / 2. \end{aligned} \quad (67)$$

The linear term coefficient is supplied by (63) with replacement of $\mathcal{R}(\mathbf{f}_{\mathbf{u}} - iw\mathbf{I})$ by $\mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_{\mathbf{u}})$.

There are three diffusional terms in the Ginzburg–Landau equation; one is given by (63), another term coefficient $c_{3,2,1}$ depends on the parametric deviation of the first-order and usually can be removed by the appropriate choice of this deviation:

$$\begin{aligned} c_{3,2,1}(\mathbf{R}_1) &= 2(\mathbf{U}^\dagger \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{U} \mathbf{R}_1) (\mathbf{U}^\dagger \mathbf{D} \mathbf{U}) / (\mathbf{U}^\dagger \mathbf{U}) \\ &- 2\mathbf{U}^\dagger \mathbf{D} \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{U} \mathbf{R}_1 \\ &+ 2(\mathbf{U}^\dagger \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_{\mathbf{u}}) \mathbf{D} \mathbf{U}) (\mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{U} \mathbf{R}_1) / (\mathbf{U}^\dagger \mathbf{U}) \\ &+ 2\mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_{\mathbf{u}}) \mathbf{D} \mathbf{U} \mathbf{R}_1. \end{aligned} \quad (68)$$

The coefficient $c_{3,1,2}$ independent of the parametric deviation has the following form:

$$c_{3,1,2} = 4(\mathbf{U}^\dagger \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_u) \mathbf{D} \mathbf{U})(\mathbf{U}^\dagger \mathbf{D} \mathbf{U}) / (\mathbf{U}^\dagger \mathbf{U}) - 4\mathbf{U}^\dagger \mathbf{D} \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_u) \mathbf{D} \mathbf{U}. \quad (69)$$

4.2.1. Hopf bifurcation

Now we turn to the case of the Hopf bifurcation for the same problem. The resulting set of equations is given by (65) with slightly changed formulae for the coefficients in the Ginzburg–Landau equation.

The modes interaction coefficient $c_{3,4}$ is calculated as shown in (66) with the only replacement of $\mathcal{R}(\mathbf{f}_u - 2k^2 \mathbf{D}(1 + \cos \alpha))$ by $\mathcal{R}(\mathbf{f}_u - 2k^2 \mathbf{D}(1 + \cos \alpha) - 2iw\mathbf{I})$, where \mathbf{I} stands for the identity matrix. Similarly, in the expression (67) for the self-interaction coefficient one must replace $\mathcal{R}(\mathbf{f}_u - 4k^2 \mathbf{D})$ by $\mathcal{R}(\mathbf{f}_u - 4k^2 \mathbf{D} - 2iw\mathbf{I})$.

The linear term coefficient again is supplied by (39) with the replacement of $\mathcal{R}(\mathbf{f}_u)$ by $\mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D} - iw\mathbf{I})$.

The diffusional coefficient $c_{3,2,1}$ depending on the parametric deviation is found as (69) with the replacement of $\mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D})$ by $\mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D} - iw\mathbf{I})$. The same replacement is valid for another diffusional coefficient $c_{3,1,2}$.

In order to perform calculation of the coefficients of the amplitude equations describing slow dynamics in the vicinity of a bifurcation point of a particular problem, values of all elements of the output of the function `BifurcationTheory` need to be specified, substitute them into the formulae and make a simplification if needed. In this section we illustrate the usage of the above results using two simple models.

4.3. Brusselator model

The first example is a well-known Brusselator model [Nicolis & Prigogine, 1977] of chemical oscillations:

$$\partial z / \partial t = a - (1 + b)z + uz^2 + (\nabla \nabla)z,$$

$$\partial u / \partial t = bz - uz^2 + d(\nabla \nabla)u.$$

The variables u , z denote concentrations of the “activator” and “inhibitor” species. This system always has a unique stationary homogeneous solution $z = a$, $u = b/a$. The dispersion relation is found as follows:

$$a^2 + a^2 k^2 + dk^2 - bdk^2 + dk^4 + iw(1 + a^2 - b + k^2 + dk^2) - w^2 = 0$$

Now we can trace two possibilities — the first is for monotonic bifurcation with frequency $w = 0$ and the second for Hopf bifurcation with nonzero w .

4.3.1. Monotonic bifurcation

We start from the determination of the bifurcation curve describing a dependence of the bifurcation parameter b on the wavenumber k and then we find the minimum of this curve $b_{cm} = (1 + a/\sqrt{d})^2$ reached at $k_{cm} = (a^2/d)^{1/4}$.

It can be seen that the monotonic bifurcation corresponds to the short-scale instability. The eigenvectors of the problem can be found as:

$$\begin{aligned} \mathbf{U} &= \left\{ \frac{ad}{a + \sqrt{d}}, 1 \right\}; \\ \mathbf{U}^\dagger &= \left\{ \frac{a + \sqrt{d}}{a}, 1 \right\}. \end{aligned} \quad (70)$$

Calculation of the coefficients of amplitude equations (65) shows that the coefficient c_{211} of the linear differential term in the first equation is equal to zero identically, the linear term is proportional to the bifurcation parameter deviation b_1 :

$$\partial_1 a_1 = - \frac{d\sqrt{d}b_1}{(a + \sqrt{d})(1 - d)} a_1.$$

Setting $b_1 = 0$ we can trivialize the above equation.

In the next order equation some of the coefficients vanish: $c_{3,2,1}(0) = 0$; $c_{3,1,1} = 0$. The coefficient of the only nonzero diffusional term in (65) is given by:

$$c_{3,1,2} = \frac{4d^2}{a(a + \sqrt{d})},$$

the linear term coefficient is proportional to second-order parametric deviation:

$$c_{3,6}(\mathbf{R}_2) = - \frac{d\sqrt{d}b_2}{a + \sqrt{d}}.$$

The dependence of the modes interaction coefficient on α is provided by:

$$\begin{aligned} c_{3,4} &= \frac{2d^2}{a(a + \sqrt{d})^2(4\cos^2 \alpha - 1)^2} \\ &\times (-8a^3 + 7a^2\sqrt{d} + 18ad - 8d\sqrt{d} \\ &+ 2a^2\sqrt{d}(-2\cos 2\alpha + \cos 4\alpha) \\ &+ 4ad(4\cos 2\alpha + \cos 4\alpha)). \end{aligned} \quad (71)$$

It can be easily seen that this coefficient diverges at $\cos \alpha = \pm 1/2$, i.e. at $\alpha = \pi/3, 2\pi/3$. The reason of the divergence is the existence of the resonance between the two modes, and for proper description one needs to incorporate the third mode with a wavevector \mathbf{k}_3 such that $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0$. The resonant cases are considered below. Finally we present the self-interaction coefficient:

$$c_{3,5} = \frac{d^2}{9a(a + \sqrt{d})^2} (-8a^3 + 5a^2\sqrt{d} + 38ad - 8d\sqrt{d}). \quad (72)$$

4.3.2. Oscillatory bifurcation

The minimum of the bifurcation curve $b_{co} = 1 + a^2$ is found at $k_{co} = 0$, which means that the oscillatory bifurcation with frequency of the limit cycle is $w = a$ that corresponds to the long-scale instability. The eigenvectors of the problem can be found as:

$$\begin{aligned} \mathbf{U} &= \left\{ -\frac{a}{a-i}, 1 \right\}; \\ \mathbf{U}^\dagger &= \left\{ \frac{a+i}{a}, 1 \right\}. \end{aligned} \quad (73)$$

The calculation produces Eqs. (33) with coefficients given by (40) and (42) with the additional diffusional term with coefficient equal to $((d+1) + ia(d-1))/2$.

It can also be noted here that by equating the critical values of the bifurcation parameter b for monotonic and oscillatory cases it is possible to find the critical value $a_c = 2\sqrt{d}/(d-1)$ at which the bifurcation is degenerate, i.e. both Hopf and Turing modes are permitted. This degenerate case will be described below.

4.4. Two-level laser model

The simple model of a two-level laser [Coullet *et al.*, 1989] describes the dynamics of the electric field interacting with an active media. The model equations are the following:

$$\begin{aligned} A_t &= ia(\nabla\nabla)A + \sigma(P - A), \\ P_t &= (1 + i\Omega)P - (R - n)A, \\ n_t &= -bn + 1/2(A^*P + AP^*). \end{aligned} \quad (74)$$

The variables A, P, n denote complex amplitude of the electrical field, complex media polarization density and real atomic population inversion, respectively.

This model exhibits short-scale oscillatory instability in the vicinity of the basic nonlasing solution $A_0 = P_0 = n_0 = 0$. It must be noted that in order to make calculations one need to complete the system (75) with complex conjugation of first two equations for A^*, P^* . As a result the state vector $\{A, A^*, P, P^*, n\}$ appears to have five components instead of the original three.

4.4.1. Oscillatory bifurcation

The bifurcation curve has a form:

$$R = 1 + \left(\frac{\Omega - ak^2}{1 + \sigma} \right)^2. \quad (75)$$

The lowest minimum (for positive a and Ω) of this curve lies at $k_c = \sqrt{\Omega/a}$ and it equals to $R_0 = 1$, the critical frequency $w_c = \Omega$. The eigenvectors of the problem are given by:

$$\mathbf{U} = \{0, 1, 0, 1, 0\}; \quad \mathbf{U}^\dagger = \left\{ 0, \frac{1}{\sigma}, 0, 1, 0 \right\}. \quad (76)$$

In this case one does not need to shift the basic solution because it does not depend on the parameters of the problem. For the calculation of the coefficients of the amplitude equations in this case one needs additional preparatory step due to the complex nature of the original problem. In the formulae for the coefficients for short-scale instabilities one may find the notion $\tilde{\mathbf{U}}$ denoting the so-called Dirac conjugated eigenvector \mathbf{U} . These vectors present particular values of the state vector, which in our case has two complex conjugated variable components. The construction of the vector $\tilde{\mathbf{U}}$ out of \mathbf{U} may be written symbolically in the form:

$$\tilde{\mathbf{U}} = \mathcal{G}(\mathbf{U}^*), \quad (77)$$

where $*$ denotes usual complex conjugation and \mathcal{G} is an operation of mutual interchange of the vector components corresponding to the complex conjugated variables. In our case the complex conjugated variables A, A^* have to be the first positions in the state vector, while P, P^* are at the next two places. As a result the vector $\tilde{\mathbf{U}}$ is constructed as:

$$\tilde{\mathbf{U}} = \{1, 0, 1, 0, 0\}.$$

The lowest-order equation for one of two excited modes with amplitudes a_1, a_2 and wavevectors

$\mathbf{k}_1, \mathbf{k}_2$ is written as:

$$\partial_1 a_1 = 2a(\mathbf{k}_1 \nabla_1) a_1 + \frac{\sigma a_1 R_1}{1 + \sigma}, \quad (78)$$

and may be simplified by setting $R_1 = 0$.

It appears that the term describing the mode-mode interaction in the Ginzburg–Landau equation in our case does not depend on the value of the angle between mode wavevectors and is given by $c_{3,4} = -2/b$; the self-interaction coefficient $c_{3,5} = -1/b$. Two out of three diffusional coefficients in the second amplitude equation are not zeros:

$$c_{3,1,1} = -\frac{ia}{\sigma}; \quad c_{3,1,2} = -\frac{4a^2}{(1 + \sigma)(1 + \sigma - i\Omega)}. \quad (79)$$

Finally the amplitude equation may be written in the form:

$$\begin{aligned} \partial_2 a_1 = & -\frac{\sigma}{b(1 + \sigma)}(2|a_2|^2 + |a_1|^2)a_1 \\ & - \frac{4a^2}{(1 + \sigma)(1 + \sigma - i\Omega)}(\mathbf{k}_1 \nabla_1)^2 a_1 \\ & - \frac{ia}{1 + \sigma}(\nabla_1 \nabla_1) a_1 + \frac{\sigma R_2}{(1 + \sigma)} a_1. \end{aligned} \quad (80)$$

5. Amplitude Equations for Convective Problems

5.1. Convective instabilities

The convective problems are characterized by the presence of the additional convective term in Eq. (52) and can be written in the following form [Rovinsky & Menzinger, 1992, 1993]:

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{u}(\mathbf{r}, t) = & \mathbf{D}(\nabla \cdot \nabla) \mathbf{u}(\mathbf{r}, t) + \varepsilon \mathbf{V}(\mathbf{n} \cdot \nabla) \mathbf{u}(\mathbf{r}, t) \\ & + \mathbf{f}(\mathbf{u}(\mathbf{r}, t), \mathbf{R}), \end{aligned} \quad (81)$$

where \mathbf{n} denotes a constant vector determining the direction of flow and the matrix \mathbf{V} sets the velocities values; it is assumed that the velocities are of the order ε . Then for the Turing instability one must call the function `BifurcationTheory` as follows:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] +
eps V.({1,0}.Nabla[r])**u -
Nabla[t]**u == 0,
u, R, t, {r,2},{r,1},{U,Ut},
{{a1,0}, {a2, alpha}}, c, eps, 2, k, 0]
```

Here the velocity direction is chosen parallel to the x -axis. Note that the small parameter of expansion ε in this case appears explicitly in the operator equation describing the problem. The result produced may be written as:

$$\begin{aligned} \partial_1 a_1 = & \frac{c_{2,1,1}}{c_{2,2}}(i\mathbf{k}_1 \nabla_1) a_1 + \frac{c_{2,3}}{c_{2,2}} a_1 + \frac{c_{2,3}(\mathbf{R}_1)}{c_{2,2}} a_1, \\ \partial_2 a_1 = & \frac{c_{3,4}}{c_{3,3}}|a_2|^2 a_1 + \frac{c_{3,5}}{c_{3,3}}|a_1|^2 a_1 + \frac{c_{3,6}}{c_{3,3}} a_1 \\ & + \frac{c_{3,6}(\mathbf{R}_1, \mathbf{R}_2)}{c_{3,3}} a_1 + \frac{c_{3,1,1}}{c_{3,3}}(\nabla_1 \nabla_1) a_1 \quad (82) \\ & + \frac{c_{3,1,2}}{c_{3,3}}(i\mathbf{k}_1 \nabla_1)^2 a_1 + \frac{c_{3,2,1}}{c_{3,3}}(i\mathbf{k}_1 \nabla_1) a_1 \\ & + \frac{c_{3,2,1}(\mathbf{R}_1)}{c_{3,3}}(i\mathbf{k}_1 \nabla_1) a_1 + \frac{c_{3,2,2}}{c_{3,3}}(\mathbf{n} \nabla_1) a_1. \end{aligned}$$

It can be noted that the set of equations is very similar to Eq. (65) with the addition of some terms. Here we write the expressions for the coefficients which are changed or added comparing with coefficients of (65). The additional linear term in the first equation is due to the velocity matrix \mathbf{V} and its coefficient is given by:

$$c_{2,3} = ik\mathbf{U}^\dagger \mathbf{V} \mathbf{U}.$$

Similarly, there are two linear terms in the second equation, their coefficients now depend on \mathbf{V} :

$$\begin{aligned} c_{3,6} = & k^2 \mathbf{U}^\dagger \mathbf{V} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{V} \mathbf{U} - k^2 (\mathbf{U}^\dagger \mathbf{V} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{V} \mathbf{U}) (\mathbf{U}^\dagger \mathbf{V} \mathbf{U}) / (\mathbf{U}^\dagger \mathbf{U}), \\ c_{3,6}(\mathbf{R}_1, \mathbf{R}_2) = & (\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_1) (\mathbf{U}^\dagger \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_1) / (\mathbf{U}^\dagger \mathbf{U}) + \mathbf{U}^\dagger \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_2 \\ & - \mathbf{U}^\dagger \mathbf{f}_{uR} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_1 \mathbf{R}_1 + \mathbf{U}^\dagger \mathbf{f}_{uRR} \mathbf{U} \mathbf{R}_1 \mathbf{R}_1 / 2 \quad (83) \\ & - ik \mathbf{U}^\dagger \mathbf{V} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_1 + ik (\mathbf{U}^\dagger \mathbf{V} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_1) (\mathbf{U}^\dagger \mathbf{V} \mathbf{U}) / (\mathbf{U}^\dagger \mathbf{U}) \\ & + ik (\mathbf{U}^\dagger \mathbf{V} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{V} \mathbf{U}) (\mathbf{U}^\dagger \mathbf{f}_{uR} \mathbf{U} \mathbf{R}_1) / (\mathbf{U}^\dagger \mathbf{U}) - ik \mathbf{U}^\dagger \mathbf{f}_{uR} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{V} \mathbf{U} \mathbf{R}_1. \end{aligned}$$

There is also additional differential term with the coefficient given by:

$$c_{3,2,1} = 2ik(\mathbf{U}^\dagger \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_u) \mathbf{VU})(\mathbf{U}^\dagger \mathbf{DU})/(\mathbf{U}^\dagger \mathbf{U}) - 2ik\mathbf{U}^\dagger \mathbf{DR}(-k^2 \mathbf{D} + \mathbf{f}_u) \mathbf{VU} + 2ik(\mathbf{U}^\dagger \mathcal{R}(-k^2 \mathbf{D} + \mathbf{f}_u) \mathbf{DU})(\mathbf{U}^\dagger \mathbf{VU})/(\mathbf{U}^\dagger \mathbf{U}) - 2ik\mathbf{U}^\dagger \mathbf{VR}(-k^2 \mathbf{D} + \mathbf{f}_u) \mathbf{DU}. \quad (84)$$

The long-scale Hopf instability case is solved by following lines:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] +
eps V.({1,0}.Nabla[r])**u- Nabla[t]**u == 0,
u, R, t, {r,2},{r,1},{U,Ut}, a, c, eps, 2, 0, w]
```

The resulting Ginzburg–Landau equation reads:

$$\partial_2 a = \frac{c_{3,4}}{c_{3,3}} |a|^2 a + \frac{c_{3,5}(\mathbf{R}_1, \mathbf{R}_2)}{c_{3,3}} a + \frac{c_{3,1,1}}{c_{3,3}} (\nabla_1 \nabla_1) a + \frac{c_{3,2,1}}{c_{3,3}} (\mathbf{n} \nabla_1) a. \quad (85)$$

Here are the coefficients of the equation:

$$\begin{aligned} c_{3,3} &= \mathbf{U}^\dagger \mathbf{U}, \\ c_{3,4} &= \mathbf{U}^\dagger \mathbf{f}_{uuu} \mathbf{UU} \tilde{\mathbf{U}}/2 - \mathbf{U}^\dagger \mathbf{f}_{uu} \mathbf{UR}(\mathbf{f}_u) \mathbf{f}_{uu} \mathbf{U} \tilde{\mathbf{U}} \\ &\quad - \mathbf{U}^\dagger \mathbf{f}_{uu} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_u - 2iw\mathbf{I}) \mathbf{f}_{uu} \mathbf{UU}/2, \\ c_{3,1,1} &= \mathbf{U}^\dagger \mathbf{DU}, \\ c_{3,2,1} &= \mathbf{U}^\dagger \mathbf{VU}. \end{aligned} \quad (86)$$

The linear term coefficient $c_{3,5}(\mathbf{R}_1)$ is given by Eq. (36).

6. Resonant and Degenerate Cases

In this section we review the most difficult cases of bifurcation analysis — resonant and algebraically degenerate bifurcations of distributed systems. We consider the three-mode resonance in the reaction–diffusion problem and demonstrate the ability of the function `BifurcationTheory` to cope with degenerate case of simultaneous existence of the Hopf and Turing bifurcations. A simple example of calculation of the amplitude equation coefficients for Brusselator model is presented. Some nontrivial examples of usage the function `BifurcationTheory` for description of resonant patterns in nonlinear optics are found in [Rubinstein & Pismen, 1997, 1998].

6.1. Three-wave resonance in Turing bifurcation

The short-scale instabilities can demonstrate resonance of normal modes, i.e. resonance of their fre-

quencies w_j and wavevectors \mathbf{k}_j :

$$\begin{aligned} \sum_j w_j &= 0; \\ \sum_j \mathbf{k}_j &= 0. \end{aligned} \quad (87)$$

The maximal number of the resonant modes is not limited, the minimal is equal to three. The simplest resonant situation arises with three monotonic modes with the wavevectors \mathbf{k}_j satisfying the condition: $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0$, i.e. the angle between the adjacent modes is $2\pi/3$. If two out of these three modes are chosen, calculations show that the coefficient of the modes interaction term given by (66) diverges [cf. Eq. (72)], and, hence, the third mode must be incorporated in order to describe the resonance properly.

6.1.1. General results

The function `BifurcationTheory` enables to generate the normal forms for resonances, in this case the values of the angles specifying the directions of the wavevectors must be set explicitly:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] -
Nabla[t]**u == 0,
u, R, t, {r,2},{r,1},{U,Ut},
{{a1,0}, {a2, 2 Pi/3}, {a3, 4 Pi/3}}, c,
eps, 2, k, 0]
```

Here we present the results produced by the function `BifurcationTheory` for the three modes resonance. These formulae may appear helpful for calculations even “by hand”.

The normal forms for the amplitude a_1 is given by (54) with additional resonant terms:

$$\begin{aligned} \partial_1 a_1 &= \frac{c_{2,1,1}}{c_{2,2}}(i\mathbf{k}_1 \nabla_1) a_1 + \frac{c_{2,4}(\mathbf{R}_1)}{c_{2,2}} a_1 + \frac{c_{2,3}}{c_{2,2}} a_2^* a_3^*, \\ \partial_2 a_1 &= \frac{c_{3,7}}{c_{3,5}} |a_3|^2 a_1 + \frac{c_{3,9}}{c_{3,5}} |a_2|^2 a_1 + \frac{c_{3,11}}{c_{3,5}} |a_1|^2 a_1 + \frac{c_{3,6}(\mathbf{R}_1)}{c_{3,5}} a_2^* a_3^* + \frac{c_{3,12}(\mathbf{R}_1, \mathbf{R}_2)}{c_{3,5}} a_1 \\ &+ \frac{c_{3,1,1}}{c_{3,5}} (\nabla_1 \nabla_1) a_1 + \frac{c_{3,1,2}}{c_{3,5}} (i\mathbf{k}_1 \nabla_1)^2 a_1 + \frac{c_{3,4,1}(\mathbf{R}_1)}{c_{3,5}} (i\mathbf{k}_1 \nabla_1) a_1 + \frac{c_{3,2,1}}{c_{3,5}} a_2^* (i\mathbf{k}_1 \nabla_1) a_3^* \\ &- \frac{c_{3,2,2}}{c_{3,5}} a_2^* (i\mathbf{k}_3 \nabla_1) a_3^* + \frac{c_{3,3,1}}{c_{3,5}} a_3^* (i\mathbf{k}_1 \nabla_1) a_2^* - \frac{c_{3,3,2}}{c_{3,5}} a_3^* (i\mathbf{k}_2 \nabla_1) a_2^*. \end{aligned} \tag{88}$$

Below there are formulae for the coefficients of the resonant terms. The quadratic term $a_2^* a_3^*$ appearing in the equation at the first time scale has the coefficient given by:

$$c_{2,3} = \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \tilde{\mathbf{U}}. \tag{89}$$

The Ginzburg–Landau equation contains three cubic terms — the self-interaction term does not change upon the addition of the third wave; two

terms describing interaction of the principal harmonic with the two others have equal coefficients $c_{3,7} = c_{3,9}$ given by (66) with an additional term:

$$2(\tilde{\mathbf{U}}^\dagger \mathbf{f}_{\mathbf{uu}} \mathbf{U} \mathbf{U})(\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \tilde{\mathbf{U}} \tilde{\mathbf{U}}) / (\tilde{\mathbf{U}}^\dagger \tilde{\mathbf{U}}). \tag{90}$$

There is a quadratic term $a_2^* a_3^*$ in the Ginzburg–Landau equation for which the coefficient is given by:

$$\begin{aligned} c_{3,6}(\mathbf{R}_1) &= \mathbf{U}^\dagger \mathbf{f}_{\mathbf{uuR}} \tilde{\mathbf{U}} \tilde{\mathbf{U}} \mathbf{R}_1 + (\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \tilde{\mathbf{U}})(\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{\mathbf{uR}} \mathbf{U} \mathbf{R}_1) / (\mathbf{U}^\dagger \mathbf{U}) \\ &+ 4(\tilde{\mathbf{U}}^\dagger \mathbf{f}_{\mathbf{uR}} \tilde{\mathbf{U}} \mathbf{R}_1)(\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \tilde{\mathbf{U}}) / (\tilde{\mathbf{U}}^\dagger \tilde{\mathbf{U}}) - 3\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{\mathbf{uR}} \tilde{\mathbf{U}} \mathbf{R}_1. \end{aligned} \tag{91}$$

There are also four differential second-order terms in the equation; their coefficients are given below.

$$c_{3,2,1} = c_{3,3,1} = 2(\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \tilde{\mathbf{U}})(\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{D} \mathbf{U}) / (\mathbf{U}^\dagger \mathbf{U}) - \mathbf{U}^\dagger \mathbf{D} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \tilde{\mathbf{U}}, \tag{92}$$

$$c_{3,2,2} = c_{3,3,2} = 4(\tilde{\mathbf{U}}^\dagger \mathbf{D} \tilde{\mathbf{U}})(\mathbf{U}^\dagger \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \tilde{\mathbf{U}}) / (\tilde{\mathbf{U}}^\dagger \tilde{\mathbf{U}}) - 2\mathbf{U}^\dagger \mathbf{f}_{\mathbf{uu}} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_u - k^2 \mathbf{D}) \mathbf{f}_{\mathbf{uR}} \mathbf{D} \tilde{\mathbf{U}}. \tag{93}$$

6.1.2. Calculations for brusselator model

The calculation of the above coefficients made with the help of the function `CalculateCoefficient` produces the following results. The coefficient of the resonant quadratic term in the lower-order equation is found as:

$$c_{2,3} = \frac{2d\sqrt{d}(\sqrt{d} - a)}{\sqrt{d} + a}.$$

The modes interaction coefficients are equal to:

$$\begin{aligned} c_{3,7} = c_{3,9} &= \frac{d^2}{a(\sqrt{d} + a)^3(d - 1)^2} \\ &\times (-3a^4 + 8a^2d + 6a^4d + d^2 - 20a^2d^2 \\ &- 3a^4d^2 + 6d^3 + 16a^2d^3 - 3d^4 + 2a\sqrt{d} \\ &\times (2a^2 + d - 2a^2d - 6d^2 + d^3)). \end{aligned}$$

The coefficients of the second-order differential terms are:

$$\begin{aligned} c_{3,2,1} = c_{3,3,1} &= \frac{4d^2}{a(\sqrt{d} + a)^2(d - 1)} \\ &\times (d + a^2d - a^2 - ad\sqrt{d}), \\ c_{3,2,2} = c_{3,3,2} &= \frac{4d^3}{a(\sqrt{d} + a)^2(1 - d)} \\ &\times (-1 + ad\sqrt{d}). \end{aligned}$$

Finally the quadratic term coefficient in the Ginzburg–Landau equation takes the form:

$$\begin{aligned} c_{3,6}(\mathbf{R}_1) &= \frac{2d^2\sqrt{d}b_1}{a(\sqrt{d} + a)^3(d - 1)^2} (2a^2 - a^2d - a^2d^2 \\ &- 3d + \sqrt{d}(ad^2 + 3ad - a)). \end{aligned}$$

6.2. Four-wave resonance in oscillatory instability

A more complicated case of the resonance arises for short-scale oscillatory instability. The simplest waves configuration contains four waves with equal frequencies w and the wavevectors making the following angles with the x -axis: $0, \alpha, \pi, \pi + \alpha$. In this case the Ginzburg–Landau equation in addition to the terms describing two-modes interaction, a term pertaining to interaction of three modes will also appear:

$$\begin{aligned} \partial_1 a_1 &= \frac{c_{2,1,1}}{c_{2,2}} (i\mathbf{k}_1 \nabla_1) a_1 + \frac{c_{2,3}(\mathbf{R}_1)}{c_{2,2}} a_1, \\ \partial_2 a_1 &= \frac{c_{3,4}}{c_{3,3}} |a_4|^2 a_1 + \frac{c_{3,6}}{c_{3,3}} |a_3|^2 a_1 + \frac{c_{3,7}}{c_{3,3}} |a_2|^2 a_1 \\ &+ \frac{c_{3,8}}{c_{3,3}} |a_1|^2 a_1 + \frac{c_{3,5}}{c_{3,3}} a_2 a_4 a_3^* \\ &+ \frac{c_{3,9}(\mathbf{R}_1, \mathbf{R}_2)}{c_{3,3}} a_1 + \frac{c_{3,1,1}}{c_{3,3}} (\nabla_1 \nabla_1) a_1 \\ &+ \frac{c_{3,1,2}}{c_{3,3}} (i\mathbf{k}_1 \nabla_1)^2 a_1 + \frac{c_{3,2,1}(\mathbf{R}_1)}{c_{3,3}} (i\mathbf{k}_1 \nabla_1) a_1. \end{aligned} \quad (94)$$

The interaction coefficient $c_{3,7}$ between two modes a_1 and a_2 with corresponding wavevectors $\mathbf{k}_1, \mathbf{k}_2$ making the angle α is given by expression:

$$\begin{aligned} c_{3,7} &= -\mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}}) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2k^2 \mathbf{D}(1 - \cos \alpha)) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2k^2 \mathbf{D}(1 + \cos \alpha)) \\ &- 2iw \mathbf{I} \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} + \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} \tilde{\mathbf{U}}. \end{aligned} \quad (95)$$

The expressions for coefficients $c_{3,6}, c_{3,4}$ can be produced out of the above by the replacements $\alpha \rightarrow \pi$ and $\alpha \rightarrow \pi + \alpha$, respectively. The self-interaction coefficient $c_{3,8}$ is found as half of the value of $c_{3,7}$ at $\alpha = 0$.

Finally, we present the expression for the three-modes interaction coefficient:

$$\begin{aligned} c_{3,5} &= -\mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2k^2 \mathbf{D}(1 + \cos \alpha)) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \tilde{\mathbf{U}} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2iw \mathbf{I}) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} \\ &- \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \mathcal{R}(\mathbf{f}_{\mathbf{u}} - 2k^2 \mathbf{D}(1 - \cos \alpha)) \mathbf{f}_{\mathbf{u}\mathbf{u}} \mathbf{U} \tilde{\mathbf{U}} \\ &+ \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{u}\mathbf{u}} \mathbf{U} \mathbf{U} \tilde{\mathbf{U}}. \end{aligned} \quad (96)$$

The calculation of the coefficients using the above results for the model of two-level laser shows that the interaction coefficients are independent of the value of the angle α : $c_{3,4} = c_{3,5} = c_{3,6} = c_{3,7} = -1/b$; the self-interaction coefficient $c_{3,8} = -1/(2b)$.

6.3. Algebraic degeneracy — Hopf–Turing bifurcation

Here we present an example of usage of the function `BifurcationTheory` for analysis of algebraically degenerated cases. Consider a situation where both Hopf and Turing bifurcations are permitted simultaneously. It may occur if the minima of the bifurcation curves for long-scale oscillatory ($k_{lo} = 0, w = w_{lo} \neq 0$) and for short-scale monotonic ($k = k_{sm} \neq 0, w_{sm} = 0$) bifurcations are at the same level.

The function is called as follows:

```
BifurcationTheory[
DD.(Nabla[r].Nabla[r])**u + f[u,R] -
Nabla[t]**u == 0,
u, R, t, {r,2}, {r,2}, {{a1,{k,0},0,U,Ut,
3}},
{a2,{0,0},w,V,Vt,2}}, c, eps, 5, {a1,a2}]
```

Here $\mathbf{U}, \mathbf{U}t$ denote the eigenvectors corresponding to the Turing mode (its amplitude $\mathbf{a}1$ is of the third-order of smallness); $\mathbf{V}, \mathbf{V}t$ correspond to the Hopf mode with second-order amplitude $\mathbf{a}2$. Scaling exponent in (58) $\alpha = 2$. The last argument of the function shows that the normal forms are produced for both modes.

The resulting equations are:

$$\begin{aligned} \partial_3 a_1 &= \frac{c_{6,2}(\mathbf{R}_3)}{c_{6,1}} a_1, \\ \partial_4 a_2 &= \frac{c_{6,4}}{c_{6,3}} |a_2|^2 a_2 + \frac{c_{6,5}(\mathbf{R}_2, \mathbf{R}_4)}{c_{6,3}} a_2 \\ &+ \frac{c_{6,1,1}}{c_{6,3}} (\nabla_1 \nabla_1) a_2. \end{aligned} \quad (97)$$

The normalization coefficients are given by:

$$\begin{aligned} c_{6,1} &= \mathbf{U}^\dagger \mathbf{U}, \\ c_{6,3} &= \mathbf{V}^\dagger \mathbf{V}. \end{aligned}$$

The linear term coefficient $c_{6,2}(\mathbf{R}_3)$ of the Turing mode is found as:

$$c_{6,2}(\mathbf{R}_3) = \mathbf{U}^\dagger \mathbf{f}_{\mathbf{u}\mathbf{R}} \mathbf{U} \mathbf{R}_3.$$

The coefficients in the normal form for the Hopf mode are given by Eqs. (35), (36) and (63) with replacements $\mathbf{U}^\dagger \rightarrow \mathbf{V}^\dagger$, $\mathbf{U} \rightarrow \mathbf{V}$, $\mathbf{R}_2 \rightarrow \mathbf{R}_4$, $\mathbf{R}_1 \rightarrow \mathbf{R}_2$.

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References

- Coulet, P., Gil, L. & Rocca, F. [1989] "Optical vortices," *Opt. Commun.* **73**, 403–408.
- Guckenheimer, J. & Holmes, P. [1983] *Nonlinear Oscillations, Dynamical Systems and Bifurcations of Vector Fields* (Springer, Berlin).
- Guckenheimer, J., Myers, M. & Sturmfels, B. [1997] "Computing Hopf bifurcations I," *SIAM J. Num. Anal.* **34**, 1–21.
- Haken, H. [1987] *Advanced Synergetics* (Springer, Berlin).
- Hale, J. K. & Koçak, H. [1991] *Dynamics and Bifurcations* (Springer, Berlin).
- Lorenz, E. N. [1963] "Deterministic nonperiodic flow," *J. Atmos. Sci.* **20**, 130–141.
- Nicolis, G. & Prigogine, I. [1977] *Self-organization in Nonequilibrium Systems, from Dissipating Structures to Order through Fluctuations* (Wiley, NY).
- Pismen, L. M. [1986] *Methods of Singularity Theory in the Analysis of Dynamics of Reactive Systems*, Lectures in Applied Mathematics **24**, Part 2, AMS p. 175.
- Pismen, L. M., Rubinstein, B. Y. & Velarde, M. G. [1996] "On automated derivation of amplitude equations in nonlinear bifurcation problems," *Int. J. Bifurcation and Chaos* **6**, 2163–2167.
- Rovinsky, A. & Menzinger, M. [1992] "Chemical instability induced by a differential flow," *Phys. Rev. Lett* **69**, 1193–1196.
- Rovinsky, A. & Menzinger, M. [1993] "Self-organization induced by the differential flow of activator and inhibitor," *Phys. Rev. Lett* **70**, 778–781.
- Rubinstein, B. Y. & Pismen, L. M. [1997] "Resonant two-dimensional patterns in optical cavities with a rotated beam," *Phys. Rev.* **A56**, 4264–4272.
- Rubinstein, B. Y. & Pismen, L. M. [1998] "Resonant patterns in a two-component optical system with 2-D feedback," *Opt. Commun.* **145**, 159–165.
- Uppal, A., Ray, W. H. & Poore, A. B. [1974] "On the dynamic behavior of continuous stirred tank reactors," *Chem. Eng. Sci.* **29**, 967–985.
- Wolfram, S. [1991] *Mathematica. A System for Doing Mathematics by Computer*, 2nd edition (Addison-Wesley).

Wolfram, S. [1996] *The Mathematica Book*, 3rd edition (Wolfram Media, Inc. and Cambridge University Press).

Appendix

Appendices contain the auxillary material showing usage of *Mathematica* for localization of the basic states and subsequent linear analysis of systems under investigation. Some examples of calculation of the coefficients of amplitude equations for particular systems are presented.

A. Linear Analysis and Amplitude Equations for Lorenz Model

We start with defining an array \mathbf{f} containing the right-hand sides of the above equations:

```
In[2]:=
Lorenz = {-sigma x + sigma y, RR x - x z -
y, x y - b z};
```

Here x , y , z denote the components of the vector \mathbf{u} and RR stands for the bifurcation parameter \mathbf{R} . The bifurcation point of the problem is determined as a point where the Jacobian matrix is singular. We find the Jacobian matrix of the problem $Lorenzmatr$ and then write a set of equations determining bifurcation points:

```
In[3]:=
Lorenzmatr = Outer[D,Lorenz,{x,y,z}];
Lorenzbifcond =
Join[Thread[Lorenz == 0],{Det[Lorenzmatr]
== 0}]
Out[3]=
{-(sigma x) + sigma y == 0,
RR x - y - x z == 0, x y - b z == 0,
-(b sigma) + b RR sigma - sigma x^2 -
sigma x y - b sigma z == 0}
```

We choose RR as the bifurcation parameter, and solve the above equations with respect to x , y , z , RR :

```
In[4]:=
Lorenzbp = First[Solve[Lorenzbifcond,
{x,y,z,RR}]]
Out[4]=
{RR -> 1, z -> 0, y -> 0, x -> 0}
```

Now it is possible to calculate the eigenvectors of the problem.


```
In[5]:=
LorenzU = First[NullSpace[Lorenzmatr /.
Lorenzbp]];
LorenzUt = First[NullSpace[Transpose
[Lorenzmatr /.
Lorenzbp]]];
```

Also a set of replacement rules required for calculation is specified:

```
In[6]:=
LorenzrU = {U -> LorenzU, Ut -> LorenzUt};
LorenzrfuR = {f[u,R] -> Lorenz};
Lorenzru = u -> {{x,0},{y,0},{z,0}};
LorenzrR = R -> {{RR, 1}};
rt1 = R[n_] -> Through[{{RR}[n]]];
```

The first of the above rules replaces the eigen-vector variables used in the formulae by their corresponding values; the next make the same for the nonlinear function $f[u,R]$. Next two rules specify the state vector variables and the bifurcation parameter with the corresponding critical values. The last rule is needed for description of the parametric deviations. Here the normalization constant is calculated using the function `CalculateCoefficient`:

```
In[8]:=
rulenorm1 = CalculateCoefficient
[Part[dynmonbif,3],
Lorenzru,LorenzrR,{w -> 0},LorenzrfuR,
LorenzrU]
Out[8]=
c[2, 1] -> 1 + 1 / sigma
```

The quadratic term coefficient (37) appears to vanish due to an inversion symmetry of the Lorenz system, the free term coefficient is calculated similarly:

```
In[9]:=
{rulequadr1,rulefree1} =
CalculateCoefficient[Part[dynmonbif,
{4,5}],
Lorenzru,LorenzrR,{w -> 0},LorenzrfuR,
LorenzrU]
Out[9]=
{c[2, 2] -> 0, c[2, 3][{RR[2]}] -> 0}
```

Now substituting the above results into the lowest-order amplitude equation one arrives to the following trivial result:

```
In[10]:=
ampeq1 = Part[dynmonbif,1] /. rt1 /.
{rulenorm1, rulequadr1, rulefree1}
Out[10]=
a(1,0)[t[1], t[2]] == 0
```

One can proceed to the next order; the main point is the calculation of the Landau coefficient of the leading term:

```
In[11]:=
rulecube2 =
CalculateCoefficient[Part[dynmonbif,7],
Lorenzru,LorenzrR,{w -> 0},LorenzrfuR,
LorenzrU]
Out[11]=
c[3, 2] -> - 1 / b
```

The linear term actually depends only on the second-order parametric deviation: $c_{34}(\mathbf{R}_2) = \mathbf{R}_2$, while the free term vanishes.

B. Linear Analysis for Brusselator Model

We define the array `Brusselator` containing the r.h.s. of the system, find the basic solution and shift it to zero:

```
In[12]:=
Brusselatororig = {a - (1 + b) z + u z^2,
b z - u z^2};
Brusselatorbasic = First[
Solve[Thread[Brusselatororig == 0],z,u]];
Brusselator =
Map[Expand, Brusselatororig /.
u -> u+b/a, z->z+a]
```

At a Hopf bifurcation point the trace of the Jacobian matrix is zero:

```
In[13]:=
Brusselatormatr = Outer[D,Brusselator,
{z,u}];
Brusselatorbifcond = Join[Thread
[Brusselator == 0],
{(Transpose[Brusselatormatr,{1,1}] /.List
-> Plus) == 0}];
Brusselatorbp = First[Solve
[Brusselatorbifcond,{z,u,b}]]
Out[13]=
{b -> 1 + a^2, u -> 0, z -> 0}
```

Now we need to determine the frequency of the limit cycle arising at the bifurcation point at which the characteristic polynomial of the Jacobian matrix equal to zero:

```
In[14]:=
Brusselatormatrbp =
Simplify[Brusselatormatr /.
Brusselatorbp];
Brusselatoreqw = CharacteristicPolynomial[
```

```

Brusselatormatrbp,x] == 0 /. x -> I w;
Brusselatorw = Last[Solve
[Brusselatoreqw,w]]
Out[14]=
{w -> a}

```

Now it is possible to calculate the eigenvectors of the problem.

```

In[15]:=
BrusselatorU = First[NullSpace
[Brusselatormatrbp -
I w IdentityMatrix[2] /. Brusselatorw]];
BrusselatorUt = First[NullSpace[Transpose
[Brusselatormatrbp -
I w IdentityMatrix[2] /. Brusselatorw]]];

```