Chapter 8
The Reaction-Diffusion Equations

Reaction-diffusion (RD) equations arise naturally in systems consisting of many interacting components, (e.g., chemical reactions) and are widely used to describe pattern-formation phenomena in variety of biological, chemical and physical systems. The principal ingredients of all these models are equation of the form

$$\partial_t \mathbf{u} = \mathbf{D}\nabla^2 \mathbf{u} + \mathbf{R}(\mathbf{u}), \tag{8.1}$$

where $\mathbf{u} = \mathbf{u}(\mathbf{r}, \mathbf{t})$ is a vector of concentration variables, $\mathbf{R}(\mathbf{u})$ describes a local reaction kinetics and the Laplace operator ∇^2 acts on the vector $\mathbf{u}$ componentwise. $\mathbf{D}$ denotes a diagonal diffusion coefficient matrix. Note that we suppose the system (8.1) to be isotropic and uniform, so $\mathbf{D}$ is represented by a scalar matrix, independent on coordinates.

8.1 Reaction-diffusion equations in 1D

In the following sections we discuss different nontrivial solutions of this system (8.1) for different number of components, starting with the case of one component RD system in one spatial dimension, namely

$$u_t = D u_{xx} + R(u), \tag{8.2}$$

where $D = \text{const}$. Suppose, that initial distribution $u(x,0)$ is given on the whole space interval $x \in (-\infty, +\infty)$.

8.1.1 The FKPP-Equation

Investigation in this field starts form the classical papers of Fisher [17] and Kolmogorov, Petrovsky and Piskunoff [25] motivated by population dynamics issues,

where authors arrived at a modified diffusion equation:

$$\partial_t u(x,t) = D\partial_x^2 u(x,t) + R(u)\,, \tag{8.3}$$

with a nonlinear source term $R(u) = u - u^2$. A typical solution of the Eq. (8.3) is a propagating front, separating two non-equilibrium homogeneous states, one of which ($u = 1$) is stable and another one ($u = 0$) is unstable [10, 13, 51]. Such fronts behavior is often said to be *front propagation into unstable state* and fronts as such are referred to as *waves (or fronts) of transition from an unstable state*.

Initially the subject was discussed and investigated mostly in mathematical society (see, e.g., [16] where nonlinear diffusion equation was discussed in details). The interest in physics in these type of fronts was stimulated in the early 1980s by the work of G. Dee and coworkers on the theory of dendritic solidification [12]. Examples of such fronts can be found in various physical [28, 52], chemical [43, 14] as well as biological [3] systems.

Notice that for Eq. (8.3) the propagating front always relaxes to a unique shape and velocity

$$c^* = 2\sqrt{D}, \tag{8.4}$$

if the initial profile is well-localized [1, 2, 50].

Numerical treatment

Let us consider Eq. (8.3) and suppose that initial distribution $u(x,0) = f(x)$ as well as no-flux boundary conditions are given. We can try to apply an implicit BTCS-method (7.13) (see Chapter 7) for the linear part of the equation, taking the nonlinearilty explicitly, i.e.,

$$\frac{u_i^{j+1} - u_i^j}{\triangle t} = D\,\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{\triangle x^2} + R(u_i^j)\,,$$

where $R(u_i^j) = u_i^j - (u_i^j)^2$. We can rewrite the last equation to the matrix form

$$A\,\mathbf{u^{n+1}} = \mathbf{u^n} + \triangle t \cdot R(\mathbf{u^n})\,, \tag{8.5}$$

where matrix A is a tridiagonal $M+1 \times M+1$ matrix of the form

$$A = \begin{pmatrix} 1+2\alpha & \boxed{-2\alpha} & 0 & \dots 0 \\ -\alpha & 1+2\alpha & -\alpha & \dots 0 \\ 0 & -\alpha & 1+2\alpha & \dots 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & \boxed{-2\alpha} & 1+2\alpha \end{pmatrix},$$

$\alpha = D\triangle t/\triangle x^2$. The boxed elements indicate the influence of no-flux boundary conditions.

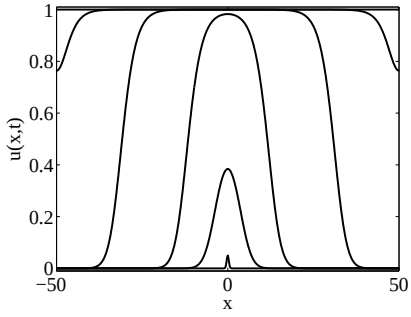

Fig. 8.1 Numerical solution of (8.3) calculated with the method (8.5) for six different time moments $t = 0, 100, 200, 400, 600, 800$.

As an example, let us solve Eq. (8.3) on the interval $x \in [-L, L]$ with the scheme (8.5). Parameters are:

`Space interval`	$L = 50$
`Space discretization step`	$\triangle x = 0.2$
`Time discretization step`	$\triangle t = 0.05$
`Amount of time steps`	$T = 800$
`Diffusion coefficient`	$D = 1$
`Initial distribution`	$f(x) = 0.05\exp(-5x^2)$

Numerical solution for six different time moments is shown on Fig. (8.1). One can see, that a small local initial fluctuation around $u = 0$ leads to an instability, that develops in a nonlinear way: a front propagates away from the initial perturbation. Finally the uniform stable state with $u = 1$ is established on the whole space interval.

8.1.2 Switching waves

Another important class of one-component RD systems is so-called *bistable systems*. They possess two stable states, say $u = u_-$ and $u = u_+$, separated by an unstable state $u = u_0$.

An example of bistable system is the Zeldovich–Frank–Kamenetsky–Equation, namely Eq. (8.2) with the reaction term

$$R(u) = u\,(1-u)\,(u-\beta)\,, \quad \beta \in (0,1)\,,$$

describing the flame propagation [54]

$$u_t = Du_{xx} + u(1-u)(u-\beta)\,, \quad \beta \in (0,1)\,. \tag{8.6}$$

The fundamental form of a pattern in bistable infinite one-component media is *a trigger wave*, which represents a propagating front of transition from one stationary state into the other. In the literature other nomenclature, e.g., *switching waves*

is also used. The propagation velocity of a flat front is uniquely determined by the properties of the bistable medium. Indeed, moving to a frame, moving with a constant velocity $\xi := x - ct$, and considering partial solution of the form $u = u(\xi)$ one obtains an equation

$$Du_{\xi\xi} + cu_{\xi} + R(u) = 0$$

with boundary conditions

$$u(\xi \to -\infty) = u_{-}, \qquad u(\xi \to +\infty) = u_{+}.$$

Introducing the potential $R(u) = \frac{\partial V(u)}{\partial u}$ one can show that in this situation the velocity of the front can be determined as [16]

$$c = \frac{V(u_{+}) - V(u_{-})}{\int\limits_{-\infty}^{+\infty} (u_{\xi})^2 d\,\xi}.$$

The numerator of the last equation uniquely defines the velocity direction. In particular, if $V(u_{+}) = V(u_{-})$ the front velocity equals zero, so *stationary front* is also a solution in bistable one-component media. However, the localized states in form of a domain, which can be produced by a connection of two fronts propagating in opposite directions, are normally unstable. Indeed, for the arbitrary choice of parameters one state ($V(u_{+})$ or $V(u_{-})$) will be dominated. This causes either collapse or expansion of the two-front solution.

Example 1: Moving fronts

Let us solve Eq. (8.6) on the interval $x \in [-L, L]$ with no-flux boundary conditions by means of numerical scheme (8.5). Other parameters are:

`Space interval`	$L = 10$
`Space discretization step`	$\triangle x = 0.04$
`Time discretization step`	$\triangle t = 0.05$
`Amount of time steps`	$T = 150$
`Diffusion coefficient`	$D = 1$

Consider four different cases, corresponding to different behaviors of the front:

a) A front moving to the right: $\beta = 0.8$;
b) A front moving to the left: $\beta = 0.1$.
   Initial distribution are:

$$u(x,0) = \begin{cases} u_{-}, & \text{for} \quad x \in [-L, 0] \\ u_{+}, & \text{for} \quad x \in (0, L]. \end{cases}$$

c) Front collision: $\beta = 0.8$;

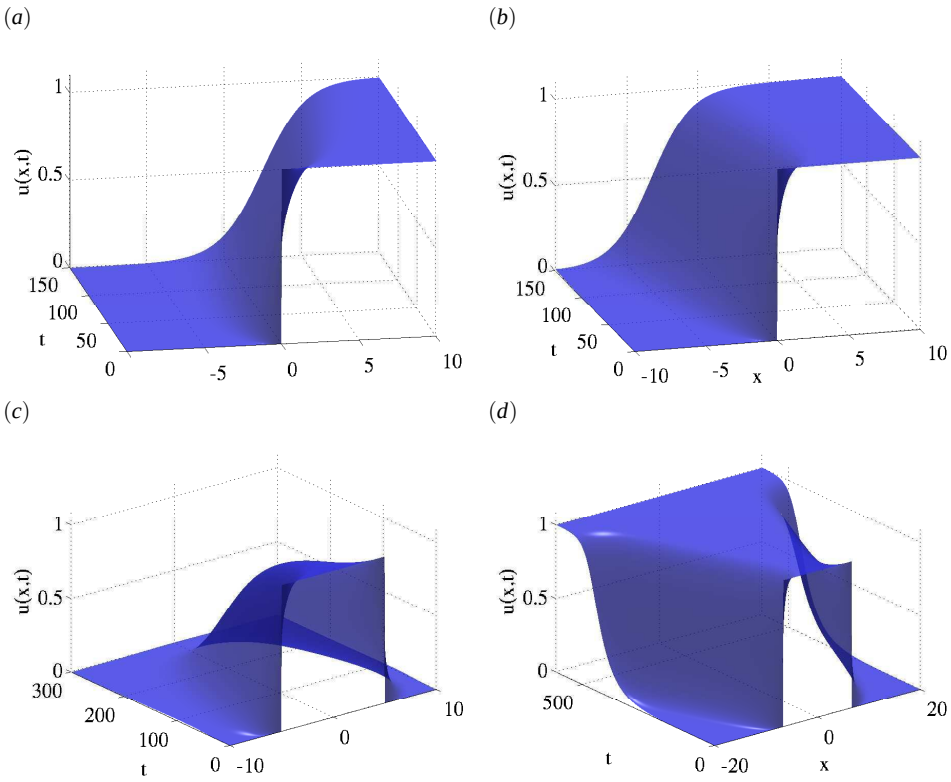

Fig. 8.2 Numerical solution of Eq. (8.6), calculated with the scheme (8.5) for four different cases: a) a front, propagating to the right for $\beta = 0.8$; b) a front, propagating to the left for $\beta = 0.1$; c) collision of two fronts, $\beta = 0.8$; d) scattering of two fronts, $\beta = 0.1$.

d) Front scattering: $\beta = 0.1$.
Initial distribution are:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \in [-L, -L/3] \\ u_+, & \text{for} \quad x \in (-L/3, L/3) \\ u_-, & \text{for} \quad x \in [L/3, L]\,. \end{cases}$$

Results of the numerical calculation is shown on Fig. 8.2.

Example 2: Stationary fronts

Now let us consider a one-dimensional RD equation (8.6), describing a bistable media for the case $\beta = -1$, i.e,

$$u_t = D u_{xx} + u(1-u^2), \qquad x \in [-L, L]. \tag{8.7}$$

Equation (8.7) has three steady state solutions: two stable $u_\pm = \pm 1$, separated with an unstable state $u_0 = 0$. One can calculate the potential values at $u = u_\pm$,

$$V(u_-) = V(u_+) \Rightarrow c = 0.$$

That is, a stationary front, connecting stable steady state is expected to be a solution of the problem. Moreover, one can constuct a localized pulse by a connection of two stable fronts. The form of the stationary front can be found analytically [16, 10], namely

$$u(x) = \tanh\left(\frac{x - x_0}{\sqrt{2D}}\right).$$

From numerical point of view one can use again the scheme (8.5) for the reaction term $R(u) = u - u^3$. That is, let us solve Eq. (8.7) on the interval $x \in [-L, L]$ with no-flux boundary conditions. Parameters are:

`Space interval`	$L = 10$
`Space discretization step`	$\triangle x = 0.04$
`Time discretization step`	$\triangle t = 0.05$
`Amount of time steps`	$T = 100$
`Diffusion coefficient`	$D = 1$

Initial distribution is:

a) A stationary front:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \le 0, \\ u_+, & \text{for} \quad x > 0. \end{cases}$$

b) A stationary pulse:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \in [-L, -L/4], \\ u_+, & \text{for} \quad x \in (-L/4, L/4), \\ u_-, & \text{for} \quad x \in [L/4, L]. \end{cases}$$

Solutions of the problem, corresponding to both cases are shown on Fig. 8.3.

8.2 Reaction-diffusion equations in 2D

8.2.1 Two-component RD systems: a Turing bifurcation

A Turing instability (or bifurcation) involves the destabilization of a homogeneus solution to form a static periodic spatial pattern (Turing pattern), whose wavelength

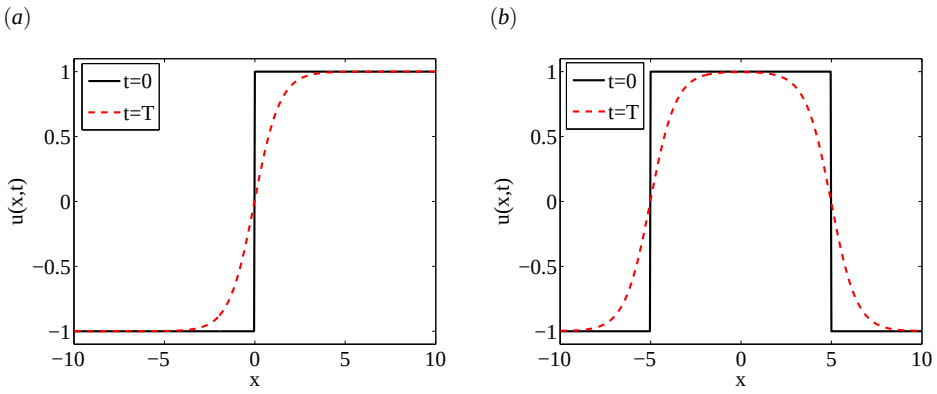

Fig. 8.3 Numerical solution of Eq. (8.7) by means of scheme (8.5): a) A stable stationary front. b) A stable stationary pulse.

depends on the local reaction kinetic parameters, diffusion coefficients of the system and is its intrinsic property. The hypothesis that just a difference in diffusion constants of components could be enough to destabilize the homogeneous solution was put forward by *A. M. Turing* in 1952 [49]. By studying the problem of biological morphogenesis he showed that a reaction-diffusion system with a different diffusion constants can autonomously produce stationary spatial patterns.

We start our analysis of Turing instability from by considering a reaction-diffusion system in general form, restricting ourself first to the case of two components, i.e.,

$$\partial_t \mathbf{u} = \mathbf{D}\nabla^2 \mathbf{u} + \mathbf{R}(\mathbf{u}) \tag{8.8}$$

where $\mathbf{u} = \mathbf{u}(\mathbf{r},\mathbf{t}) = (u,v)^T$ is a vector of concentration variables, $\mathbf{R}(\mathbf{u}) = (f(u,v), g(u,v))^T$ describes as before a local reaction kinetics and the Laplace operator ∇^2 acts on the vector $\mathbf{u}$ componentwise. $\mathbf{D}$ denotes a diagonal diffusion coefficient matrix,

$$\mathbf{D} = \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix}.$$

Let $\mathbf{u_0} = (u_0, v_0)^T$ be a homogeneous solution (or steady-state solution) of the system (8.8), i.e. $f(u_0, v_0) = g(u_0, v_0) = 0$. Suppose that this solution is stable in absence of diffusion, namely the real parts of all eigenvalues of the Jacobi matrix

$$\mathbf{A} = (\partial \mathbf{R}/\partial \mathbf{u})_{\mathbf{u}=\mathbf{u_0}} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix},$$

describing the local dynamics of the system (8.8) are less that zero. For the case of a 2×2 matrix this is equivalent to the simple well-known condition for the trace and the determinant of the matrix $\mathbf{A}$ (Vieta's formula), namely

$$\begin{aligned} \mathrm{Sp}(\mathbf{A}) &= \lambda_1 + \lambda_2 = f_u + g_v < 0\,, \\ \det(\mathbf{A}) &= \lambda_1\lambda_2 = = f_u g_v - f_v g_u > 0\,. \end{aligned} \tag{8.9}$$

Keeping Eq. (8.9) in mind, let us see if the presence of diffusion term can change the stability of $\mathbf{u_0}$. To this end, consider a small perturbation $\tilde{\mathbf{u}}$, i.e. $\mathbf{u} = \mathbf{u_0} + \tilde{\mathbf{u}}$ and the corresponding linear equation for it:

$$\partial_t \tilde{\mathbf{u}} = \mathbf{D}\nabla^2\tilde{\mathbf{u}} + \mathbf{A}\tilde{\mathbf{u}}\,. \tag{8.10}$$

After decomposition $\tilde{\mathbf{u}}$ into modes $\tilde{\mathbf{u}} \sim \mathbf{a_k} e^{ikr}$ we get the equation

$$\dot{\mathbf{a}}_\mathbf{k} = \mathbf{B}\mathbf{a}_\mathbf{k}\,, \tag{8.11}$$

where $\mathbf{B} = \mathbf{A} - k^2\mathbf{D}$.

As mentioned above, the stability conditions for the system (8.11) with a 2×2 matrix $\mathbf{B}$ can be written as:

$$\begin{aligned} \mathrm{Sp}(\mathbf{B}) &< 0 \quad \forall k\,, \\ \det(\mathbf{B}) &> 0 \quad \forall k\,, \end{aligned} \tag{8.12}$$

where

$$\mathrm{Sp}(\mathbf{B}) = -(D_u + D_v)\,k^2 + \mathrm{Sp}(\mathbf{A})\,, \tag{8.13}$$

$$\det(\mathbf{B}) = D_u D_v k^4 - (D_u g_v + D_v f_u)\,k^2 + \det(\mathbf{A})\,. \tag{8.14}$$

Notice, that for $k = 0$ the conditions (8.12) are equivalent to the stability criterion (8.9) for the local dynamics. In particular this implies that $\mathrm{Sp}(\mathbf{B}) < 0$ for all k (see gray curve in Fig. 8.4 for illustration), so the instability of the homogeneous solution can occur only due to violation of the second condition (8.12), that is, $\det(\mathbf{B})$ should be equal to zero for some k. It means that the instability occur at the point where the equation $\det(\mathbf{B}) = 0$ has a multiple root. To find it we can simply calculate a minimum of the function $T(k) = \det(\mathbf{B})$:

$$T'(k) = 4D_u D_v k^3 - 2(D_u g_v + D_v f_u)k = 0 \quad \Rightarrow \quad k^2 = \frac{1}{2}\left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right).$$

From the last equation can be seen that the situation described above is possible if

$$D_u g_v + D_v f_u > 0\,. \tag{8.15}$$

In this case the critical wavenumber is

$$k_c = \sqrt{\frac{1}{2}\left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)} \tag{8.16}$$

and instability occurs on condition that

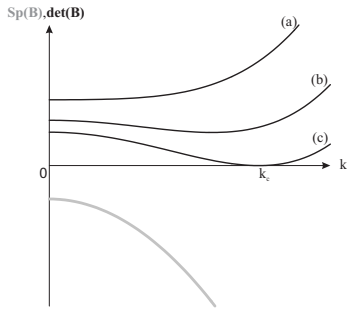

Fig. 8.4 Three different cases of dependence of the function $T(k) = \det(\mathbf{B})$ on the wave vector k are presented. (a) the function $T(k)$ has no roots, so the stability of $\mathbf{u_0}$ is not affected as well as in the case (b). $T(k) > 0$ for all k, but minimum of this function exists. (c) $T(k) = 0$ for $k = k_c$, indicating the onset of instability.

$$T(k_c) \leq 0 \quad \Leftrightarrow \quad k_c^4 = \left(\frac{1}{2}\left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)\right)^2 > \frac{\det\mathbf{A}}{D_u D_v}\,. \tag{8.17}$$

The instability scenario, described above is illustrated in Fig. 8.4, where three different cases of dependence of the function $T(k) = \det(\mathbf{B})$ on the wave vector k are presented. In Fig. 8.4 (a) the function $T(k)$ has no roots, so the stability of $\mathbf{u_0}$ is not affected as well as in the case (b). Here $T(k) > 0$ for all k, but minimum of this function exists. Finally, in Fig. 8.4 (c) $T(k) = 0$ for $k = k_c$, indicating the onset of instability.

Hence, the full system of the conditions for instability of the homogeneous solution $\mathbf{u_0}$ is

$$\boxed{\begin{aligned} f_u + g_v &< 0\,, \\ f_u g_v - f_v g_u &> 0\,, \\ D_u g_v + D_v f_u &> 0\,, \\ \left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)^2 &> \frac{4\det\mathbf{A}}{D_u D_v}\,. \end{aligned}} \tag{8.18}$$

A detailed description of the mechanism of Turing instability can also be found in [32, 31, 23].

While the conditions for the onset of a Turing bifurcation are rather simple, the determination of the nature of the pattern that is selected is a more difficult problem since beyond the bifurcation point a finite band of wavenumbers is unstable. Pattern selection is usually approached by studying *amplitude equations* that are valid near the onset of the instability. To determine which modes are selected, modes and their complex conjugates are usually treated in pairs so that the concentration field, expanded about the homogeneous solution, reads

$$\mathbf{u}(\mathbf{r},t) = \mathbf{u_0} + \sum_{j=1}^{n} \left(A_j(t) e^{i\mathbf{k_j}\mathbf{r}} + c.c.\right),$$

where $\mathbf{k_j}$ are different wavevectors such that $|\mathbf{k_j}| = k_c$. In one dimensional space the situation is rather simple, as result of the instability is represented by a periodic in

space structure. In two space dimension this form leads to *stripes* for $n = 1$, *rhombi* (or *squares*) for $n = 2$ and *hexagons* for $n = 3$. The pattern and wavelength that is selected depends on coefficients in the nonlinear amplitude equation for the complex amplitude A_j, but some conclusions about selected pattern can be made using, e.g., symmetry arguments. In particular, in the case of hexagonal pattern, in which three wave vectors are mutually situated at an angle of $2\pi/3$, i.e., $\mathbf{k_1} + \mathbf{k_2} + \mathbf{k_3} = 0$, the absence of inversion symmetry ($\mathbf{u} \mapsto -\mathbf{u}$) leads to additional quadratic nonlinearity in the amplitude equation. The latter, in its turn, ends in a fact, that hexagonal pattern has the maximum growth rate near the threshold and is therefor preferred (for details see [10]).

The general procedure in details for the derivation of such amplitude equations based on mode projection techniques can be found in [19]. Another approach, using multi scale expansion was evolved in [33].

8.2.1.1 The Brusselator Model

The Brusselator model is a classical reaction-diffusion system, proposed by I. Prigogine and co-workers in Brussels in 1971 [18, 34]. The model describes some chemical reaction with two components

$$u_t = D_u \triangle u + a - (b+1)\,u + u^2 v, \tag{8.19}$$
$$v_t = D_v \triangle v + b\,u - u^2 v. \tag{8.20}$$

Here $u = u(x,y,t)$, $v = v(x,y,t)$, a, b are posotive constants. The steady state solution is

$$u_0 = a\,, \quad v_0 = \frac{b}{a}\,.$$

For the system (8.19) the matrices $\mathbf{D}$, $\mathbf{A}$ and $\mathbf{B}$ are given by

$$\mathbf{D} = \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix},$$

and

$$\mathbf{B} = \begin{pmatrix} b-1-D_u k^2 & a^2 \\ -b & -D_v k^2 - a^2 \end{pmatrix}.$$

Suppose that the system (8.19) is local stable, i.e.,

$$\mathrm{Sp}(\mathbf{A}) = b - 1 - a^2 < 0\,,$$
$$\mathrm{Det}(\mathbf{A}) = -(b-1)\,a^2 + a^2 b = a^2 > 0\,.$$

Note that the violation of the first condition above leads to tthe Hopf bifurcation, i.e., the onset of Hopf instability is

$$\boxed{\mathrm{Sp}(\mathbf{A}) \geq 0 \Leftrightarrow b \geq b_H = 1 + a^2\,.}$$

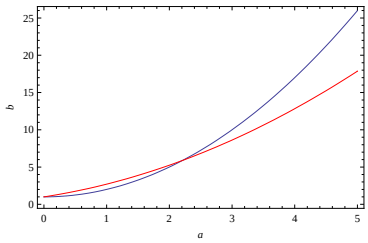

Fig. 8.5 Bifurcation diagram in (a, b) parameter space, indicating the onset of Hopf (blue line) and Turing (red line) instabilities. Here $D_u = 5$, $D_v = 12$.

The critical wavenumber is

$$k_c = \sqrt{\frac{1}{2}\left(\frac{b-1}{D_u} - \frac{a^2}{D_v}\right)}.$$

The existence of k_c is equivalent to the following condition

$$b > 1 + \frac{D_u}{D_v}a^2 + 1 \Rightarrow \frac{D_u}{D_v} < 1.$$

The instability occurs, if

$$\mathrm{Det}(\mathbf{B}(k_c)) \leq 0 \Leftrightarrow b > b_T = \left(1 + a\sqrt{\frac{D_u}{D_v}}\right)^2.$$

Hence, the conditions (8.18) for the system (8.19) takes the form

$$\boxed{\begin{array}{l} b < b_H = 1 + a^2, \\ b > b_T = \left(1 + a\sqrt{\dfrac{D_u}{D_v}}\right)^2, \\ \dfrac{D_u}{D_v} < 1. \end{array}} \tag{8.21}$$

On Fig. 8.5 both b_H (blue line), b_T (red line) as functions of a are shown. The thresholds of these two instabilities coincide at codimensional-two Turing-Hopf point $b_H = b_T$

$$a_c = \frac{2\sqrt{\sigma}}{1-\sigma},$$

where $\sigma = D_u/D_v$.

From a numerical point of view, one can apply the scheme (7.19), taking the nonlinear terms explicitly. Parameters are

`Space interval`	$L = 50$
`Space discretization step`	$\triangle x = 0.5$
`Time discretization step`	$\triangle t = 0.05$
`Amount of time steps`	$T = 4000$
`Diffusion coefficients`	$D_u = 5, D_v = 12$
`Reaction kinetics`	$a = 3, b = 9$

The result of calculation is shown on Fig. 8.6. The uniform state becomes unstable in favor of finite wave number perturbation. That is, starting with random perturb homogeneous solution (see Fig. 8.6 (a)) one obtains a high-amplitude stripe pattern, shown in Fig. 8.6 (c).

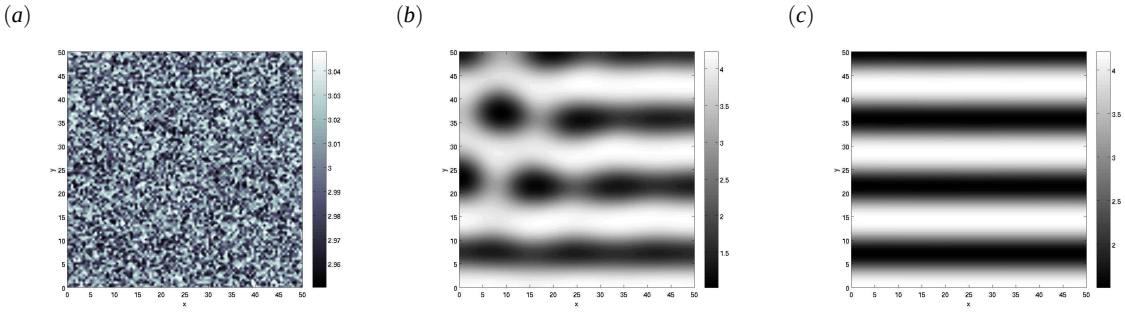

Fig. 8.6 Stripe pattern, obtained as a numerical solution of Eq. (8.19) by means of the modified ADI scheme (7.19) for three different time moments: a) $t = 0$; b) $t = 2000$; c) $t = 4000$.