Chapter 4
Reaction–Diffusion Fronts

Traveling waves are typical nonequilibrium phenomena encountered in numerous instances in physics, chemistry, biology, and other areas [129, 82, 309, 310]. Reacting and diffusing systems described by the RD equation (2.3) represent a particular well-studied class of applications. Equation (2.3) is known as Fisher's equation, if the reaction term has the logistic form $F(\rho) = r\rho(1-\rho)$:

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} + r\rho(1-\rho). \tag{4.1}$$

It was introduced in 1937 in the seminal contributions of R. A. Fisher [132] and A. N. Kolmogorov, together with I. G. Petrovskii and N. S. Piskunov [232] as a model for the spreading of an advantageous gene. Consequently, we will refer to (4.1) also as the FKPP equation. It is the simplest and most well-known equation that has traveling wave solutions.

4.1 Propagating Fronts

A *front* corresponds to a traveling wave solution, which maintains its shape, travels with a constant velocity v^*, $\rho(x,t) = \rho(x - v^* t)$, and joins two steady states of the system. The latter are uniform stationary states, $\rho(x,t) = \overline{\rho}$, where $F(\overline{\rho}) = 0$. For the logistic kinetics, the steady states are $\overline{\rho}_1 = 0$ and $\overline{\rho}_2 = 1$. While the logistic kinetics has only two steady states, three or more stationary states can exist for a broad class of systems in nonlinear chemistry and population dynamics with Allee effect, but a front can only connect two of them. To determine the propagation direction of the front, we need to evaluate the stability of the stationary states, see Sect. 1.2. The steady state $\overline{\rho}$ is stable if $F'(\overline{\rho}) < 0$ and unstable if $F'(\overline{\rho}) > 0$. Let the initial particle density $\rho(x,0)$ be such that on a certain finite interval, $\rho(x,0)$ is different from 0 and 1, and to the left of this interval $\rho(x,0) = 1$, while to the right $\rho(x,0) = 0$. In this case, the initial condition is said to have compact support. Kolmogorov et al. [232] showed for Fisher's equation that due to the combined effects of diffusion and reaction, the region of density close to 1 expands to the

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right. There exists a front that connects the stable steady state to the unstable steady state and that propagates to the right; the stable state invades the unstable state.

Consider a general reaction term that satisfies $F(0) = F(1) = 0$. If F vanishes at $\rho = c > 0$ with $c \neq 1$, ρ can be renormalized by defining a new field ρ/c for which the above condition is satisfied. Aronson and Weinberger [18] showed that any positive, sufficiently localized (this means decaying faster than exponentially for $|x| \to \infty$) initial condition $\rho(x, 0)$, with $\rho(x, 0) \in [0, 1]$, evolves into a front propagating with velocity v^*, i.e., for large t, $\rho(x, t)$ behaves as $\rho(x - v^*t)$. The shape of the front is determined by the boundary value problem

$$D\rho_{zz} + v\rho_z + F(\rho) = 0 \tag{4.2}$$

with

$$\lim_{z\to-\infty} \rho(z) = 1 \quad \text{and} \quad \lim_{z\to+\infty} \rho(z) = 0. \tag{4.3}$$

Here $z \equiv x - vt$, and (4.2) is obtained by transforming (2.3) to the frame co-moving with the front, since $\partial_x\rho \to \mathrm{d}\rho/\mathrm{d}z \equiv \rho_z$ and $\partial_t\rho \to -v\mathrm{d}\rho/\mathrm{d}z \equiv -v\rho_z$. Aronson and Weinberger [18] characterized the asymptotic velocity v^* as the minimum value of the parameter v in (4.2) for which the solution $\rho(z)$ is monotonic. This poses the problem of how to determine the value of v^* for different reaction terms. We will consider two types of reaction terms.

Case A: $F'(0) > 0$, $F(\rho) > 0$, $\rho \in (0, 1)$. This case is known as heterozygote intermediate in population dynamics or as KPP kinetics.

Case B: $F(\rho) > 0$ for all $\rho \in (b, 1)$ and $F(\rho) < 0$ for all $\rho \in (0, b)$ with $b \in (0, 1)$, $\int_0^1 F(\rho)\mathrm{d}\rho > 0$, and $F'(0) < 0$. This case is known as heterozygote inferior in population dynamics or as bistable kinetics.

In both cases, (4.2) can be viewed as Newton's equation for a particle moving in one dimension under the action of the force $-F(\rho) - v\rho_z$; the variable z plays the role of time. The force $-F(\rho)$ is conservative and derives from the potential $V(\rho) = \int_0^\rho F(s)\mathrm{d}s$.

If the kinetic term $F(\rho)$ belongs to Case A, the potential has a minimum at the point $\rho = 0$ and a maximum at $\rho = 1$. The second term, $-v\rho_z$, in (4.2) represents a damping force, where v represents the viscosity. Then (4.2) describes the motion of a particle rolling down from the top of the potential at $\rho = 1$ to the bottom of the potential well, $\rho = 0$, in the presence of a viscous force. If v is small, i.e., the viscosity is small, the particle oscillates near the bottom of the well before it settles down at the minimum $\rho = 0$. If v increases, there exists a threshold value at which the oscillations cease. In other words, the particle rolls down monotonically from $\rho = 1$ to $\rho = 0$; in mechanics this is known as critical damping. If v increases even further, the particle continues to roll down monotonically and has less and less velocity at every point of its trajectory. Consequently, there exists a critical value of v, which we denote by v^*, such that for $v \geq v^*$, there will be monotonically decreasing solutions to (4.2). The front is said to be *propagating into the* *unstable state*. This result was proven rigorously by Aronson and Weinberger, who also showed that the critical value v^* is the front velocity for the RD equation in Case A, if the front evolves from an initial condition with compact support.

If $F(\rho)$ belongs to Case B, the potential has two maxima, at $\rho = 1$ and $\rho = 0$, and a minimum at $\rho = b$. The particle starts at $\rho = 1$, $z = -\infty$, and needs to arrive at $\rho = 0$, $z = +\infty$, with zero velocity. Energy conservation requires that the height of the maximum at $\rho = 0$ must be smaller than the height of the maximum at $\rho = 1$. Otherwise the particle never reaches $\rho = 0$. This condition is precisely $\int_0^1 F(\rho)\mathrm{d}\rho > 0$. In this case, the front connects two stable states and is said to be *propagating into a metastable state*; $\rho = 0$ is less stable than $\rho = 1$. It should be clear intuitively that there is only one value of v^* for which the particle rolls down from $\rho = 1$ to the bottom of the valley at $\rho = b$ and then climbs up to the top at $\rho = 0$ to stop there with zero velocity. If $v < v^*$, the particle overshoots at $\rho = 0$, leading to an unphysical front. If $v > v^*$, the particle becomes trapped forever at $\rho = b$, representing again a front propagating into an unstable state. We represent schematically this discussion in Fig. 4.1.

A phase plane analysis represents a useful alternative to the mechanical analogy discussed above. The phase plane is constructed by the standard technique of converting the second-order ordinary differential equation (4.2) into a system of two first-order differential equations:

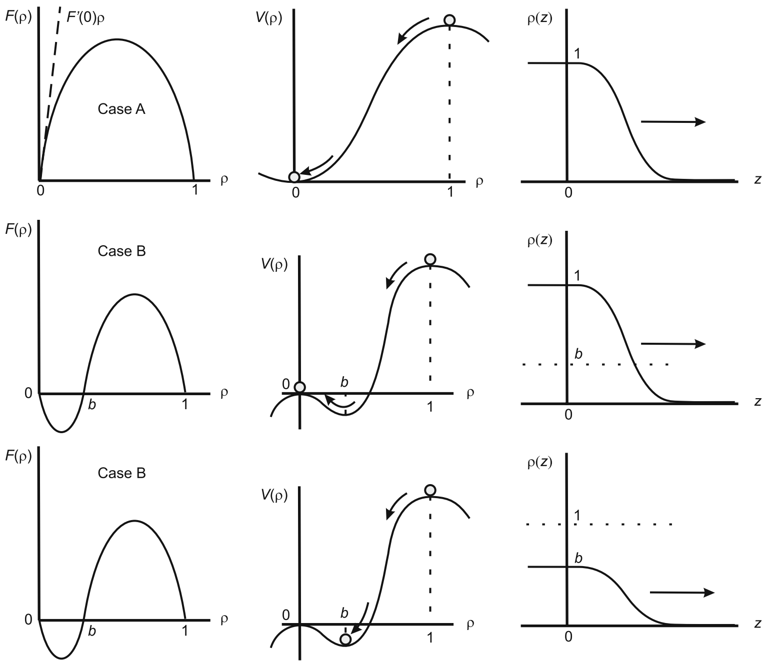

Fig. 4.1 Schematic picture for Cases A and B. We plot the reaction term, its corresponding potential, and the front profile

$$\rho_z = -q, \tag{4.4a}$$
$$q_z = -\frac{v}{D}q - \frac{r}{D}F(\rho). \tag{4.4b}$$

In the phase plane (ρ, q), a front corresponds to trajectory that connects two steady states of (4.4). Such a trajectory is know as a *heteroclinic orbit* or a heteroclinic connection. The steady states of (4.4) are given by $(\overline{\rho}, 0)$, where $F(\overline{\rho}) = 0$. The phase plane trajectories or orbits of (4.4) are the solutions of

$$\frac{\mathrm{d}\rho}{\mathrm{d}q} = \frac{vq + rF(\rho)}{Dq}. \tag{4.5}$$

To be specific, we consider logistic kinetics and Nagumo kinetics [274], $F(\rho) = r\rho(1-\rho)(\rho-b)$, as examples for cases A and B, respectively. For the logistic case, a linear stability analysis of the stationary states (0, 0) and (1, 0) provides their eigenvalues $\lambda_\pm(0,0) = -v/2 \pm \sqrt{v^2 - 4Dr}/2$ and $\lambda_\pm(1,0) = -v/2 \pm \sqrt{v^2 + 4Dr}/2$, respectively. The state (0, 0) is a stable node if $v > 2\sqrt{Dr}$ and a stable focus if $v < 2\sqrt{Dr}$. The state (1, 0) is always a saddle point. To be physically acceptable, a front must always be nonnegative. Consequently, only nonnegative heteroclinic orbits are acceptable. Such orbits can only exist if (0, 0) is a stable node. In other words, fronts only exist for $v > 2\sqrt{Dr}$. Since there exists a heteroclinic connection or front for each value of v with $v > 2\sqrt{Dr}$, this analysis does not yield a unique propagating velocity. In fact, the front velocity v depends on the initial condition, specifically on the tail of the initial condition.

For bistable kinetics there exist three steady states: (0, 0), $(b, 0)$, and (1, 0). Both (0, 0) and (1, 0) are saddle points, while $(b, 0)$ is stable. A heteroclinic connection between (1, 0) and $(b, 0)$ requires $(b, 0)$ to be stable node, which is satisfied for $v > 2\sqrt{b(1-b)}$. This case is equivalent to the logistic case. The heteroclinic orbit corresponding to a front connecting (0, 0) and (1, 0) must be a saddle–saddle connection. If one fixes b and varies v, one finds that for low values of v the phase plane trajectories undershoot the state (1, 0), while for large values of v, the phase plane trajectories overshoot the state (1, 0). There is a unique saddle–saddle connection, the separatrix, which is uniquely determined by a specific value of v. In contrast to the logistic case, where an infinite number of fronts exist if v is larger than $2\sqrt{Dr}$, only a single front with a unique velocity exists in the bistable case. In Fig. 4.2 we depict the phase portrait for both the logistic and the bistable cases. In the next two sections, we present quantitative methods to characterize front propagation for both cases A and B.

4.1.1 Fronts Propagating into Unstable States. Pulled vs Pushed Fronts

Consider the RD equation (2.3). Without specifying the shape of $F(\rho)$, we assume two steady states such that

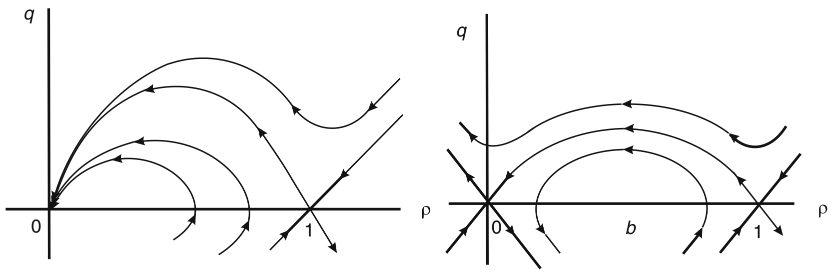

Fig. 4.2 Phase portrait for logistic and bistable reaction terms. The front is a heteroclinic saddle–node connection for the logistic case. The front is a saddle–saddle connection for the bistable case

$$F(0) = F(1) = 0 \quad \text{and} \quad F(\rho) > 0, \text{ if } 0 < \rho < 1, \tag{4.6}$$

i.e., $\overline{\rho} = 0$ is an unstable steady state and $\overline{\rho} = 1$ a stable steady state. We linearize the RD equation in the frame comoving with the front around the unstable steady state:

$$D\rho_{zz} + v\rho_z + F'(0)\rho = 0. \tag{4.7}$$

Looking for exponential solutions, we find $\rho(z) \sim A\mathrm{e}^{-\lambda_+ z} + B\mathrm{e}^{-\lambda_- z}$, where

$$\lambda_\pm = \frac{v}{2} \pm \frac{1}{2}\sqrt{v^2 - 4DF'(0)}. \tag{4.8}$$

The solutions are physically acceptable if

$$v \geq 2\sqrt{DF'(0)}. \tag{4.9}$$

Otherwise the solution oscillates around the state $\rho = 0$, resulting in negative values for the particle density. The linear analysis establishes the existence of a minimum value for the front velocity. We can also obtain the minimum value by substituting $\rho(z) \sim \mathrm{e}^{-\lambda z}$ in (4.7), writing the characteristic equation in the form

$$v(\lambda) = D\lambda + \frac{F'(0)}{\lambda}, \tag{4.10}$$

and calculating

$$v^* = \min_\lambda [v(\lambda)] = 2\sqrt{DF'(0)}. \tag{4.11}$$

Aronson and Weinberger [18] obtained the condition

$$2\sqrt{DF'(0)} \leq v^* < 2\sqrt{D \sup_\rho \left[\frac{F(\rho)}{\rho}\right]}, \tag{4.12}$$

for fronts evolving from initial conditions with compact support. This result provides both a lower and an upper bound for the front velocity. For any concave kinetic term, i.e., $F(\rho) \leq \rho F'(0)$, the lower and the upper bounds in (4.12) coincide, and the front velocity can be predicted with certainty:

$$v^* = 2\sqrt{DF'(0)}. \tag{4.13}$$

It equals the minimum velocity obtained by linearizing around the unstable state, the linear velocity. In this case the front dynamics is determined by the $\rho(x,t) \approx 0$ region. The front is called a *pulled* front, since it is pulled by its leading edge. The lower and upper bounds do *not* coincide for convex kinetic terms, and the front velocity is larger than the linear velocity. In this case, the nonlinear part of the kinetic term plays an important role in determining the value of the front velocity; the front dynamics is *pushed* by its interior part.

We consider the Ginzburg–Landau reaction term $F(\rho) = \rho(1-\rho)(1+\alpha\rho)$, with $\alpha > 0$, in (2.3) to illustrate the existence of pulled and pushed regimes. This RD equation has two steady states, $\overline{\rho} = 0$ (unstable) and $\overline{\rho} = 1$ (stable). The front connecting both states propagates into the unstable state, which resembles the situation in the FKPP case. However, Ben-Jacob et al. [37] show that when the front emerges from initial conditions with compact support, the velocity is given by

$$v = \begin{cases} 2\sqrt{D}, & \alpha \leq 2, \\ \left(\sqrt{\alpha} + 2/\sqrt{\alpha}\right)\sqrt{D/2}, & \alpha > 2. \end{cases} \tag{4.14}$$

The linear velocity $2\sqrt{D}$ is selected by the front only if $\alpha \leq 2$. The front is pulled in this case. However, if $\alpha > 2$, the selected velocity is $\left(\sqrt{\alpha} + 2/\sqrt{\alpha}\right)\sqrt{D/2}$, and the front is pushed. The value $\alpha = 2$ corresponds to the transition between pulled and pushed regimes.

The asymptotic velocity depends explicitly on the shape of the initial conditions, if they do not have compact support. An adaptation of the Hamilton–Jacobi theory from classical mechanics is a useful technique to deal with this problem in a very general way, see below. The prototypical example of a concave reaction term is the KPP or logistic term $F(\rho) = r\rho(1-\rho)$. Equation (4.13) implies that $v = 2\sqrt{rD}$. Examples for convex reaction functions typically occur in combustion theory, where $F(\rho) = \mathrm{e}^{-\rho_c/\rho}(1-\rho)$ is referred to as the Arrhenius reaction term, or $F(\rho) = \rho^m(1-\rho)$ for forest fire models. In these cases, as well as for Case B, generally the variational characterization is the only tool that can provide analytical expressions for the front velocity. Other types of reaction terms are a combination of Cases A and B, such that the kinetic term is convex for a range of values of ρ, while elsewhere it is concave.

4.1.2 Transient Dynamics of Pulled Fronts

Pushed fronts, such as fronts propagating into a metastable state, converge exponentially to the asymptotic front profile $\rho(x - vt)$. Both the profile and velocity of pulled fronts converge algebraically. It was proven rigorously by Bramson [57] that the solution of the Fisher equation with a KPP reaction term relaxes to a unique front profile $\rho(x - 2t)$, where the velocity converges asymptotically as $v(t) = 2 - \frac{3}{2t}$. (Here and in the remainder of this section, we consider the case that space and time have been scaled such that $D = r = 1$.) More recently, Ebert and van Saarloos [103, 104] found universal behavior in the relaxation to the asymptotic regime for fronts emerging from initial conditions with compact support or with exponential decay. We summarize their main results for the first case. We consider the shape of the transient front as a small perturbation η about the asymptotic shape, $\rho^*[x-v(t)t]$, where $v(t) = v^*+\dot{X}(t)$. Then, written in the frame $\xi = x-v^*t-X(t)$, the Fisher equation (2.3) with logistic growth reads

$$\rho(\xi, t) = \rho^*(\xi) + \eta(\xi, t) = \rho^*(\xi) + \dot{X}(t)\eta_s(\xi) \tag{4.15}$$

for the interior region of the front, $\xi \ll 2\sqrt{t}$. Here $\eta(\xi, t)$ obeys the equation

$$\frac{\partial \eta}{\partial t} = \mathcal{L}^*\eta + \dot{X}(t)\frac{\partial}{\partial \xi}\left[\eta + \rho^*(\xi)\right] + \frac{\eta^2}{2}F''(\rho^*) + O(\eta^3), \tag{4.16}$$

with $\mathcal{L}^* = \partial_\xi^2 + v^*\partial_\xi + F'(\rho^*)$. The fact that $\dot{X}(t)$ is $O(t^{-1})$ suggests the asymptotic expansion

$$\dot{X}(t) = \frac{c_1}{t} + \frac{c_{3/2}}{t^{3/2}} + \cdots, \tag{4.17}$$

$$\eta(\xi, t) = \frac{\eta_1}{t} + \frac{\eta_{3/2}}{t^{3/2}} + \cdots. \tag{4.18}$$

Substitution of this expansion into (4.16) yields the hierarchy of ordinary differential equations:

$$\mathcal{L}^*\eta_1 = -c_1\partial_\xi\rho^*, \quad \mathcal{L}^*\eta_{3/2} = -c_{3/2}\partial_\xi\rho^*, \ldots. \tag{4.19}$$

Each η_i is determined by its differential equation, the requirement $\eta_i(0) = 0$, and the appropriate boundary conditions. The equations for η_1/c_1 and $\eta_{3/2}/c_{3/2}$ are precisely the differential equations for $\eta_s(\xi)$ in (4.16).

In the far edge, where $\xi \geq O(\sqrt{t}) \gg 1$, a different expansion is needed, as the transient profile falls off faster than ρ^*, so that $\eta \approx -\rho^*$. Linearizing about $\rho = 0$ one finds

$$\rho(\xi, t) = \mathrm{e}^{-\xi-\xi^2/(4t)} \left[\sqrt{t} g_{-1/2}\left(\frac{\xi^2}{4t}\right) + g_0\left(\frac{\xi^2}{4t}\right) + \frac{g_{1/2}\left(\frac{\xi^2}{4t}\right)}{\sqrt{t}} + \cdots \right], \tag{4.20}$$

where the functions g_i obey a new hierarchy of ordinary differential equations that can also be integrated with the appropriate boundary conditions. Finally, matching this solution to the one for the interior region, we determine the parameters c_1 and $c_{3/2}$, and the front velocity is found to be

$$v(t) = v^* - \frac{3}{2t} + \frac{3\sqrt{\pi}}{2t^{3/2}} + \cdots. \tag{4.21}$$

4.1.3 Front Propagation into Metastable States

As explained above, the shape and velocity of a front propagating into a metastable state is governed by the nonlinear (interior) part, and the nonlinear term in the reaction function plays an important role. When a front propagates into a metastable state, only one velocity is possible, in contrast to a front propagating into an unstable state. In the latter case, there exists an infinite number of possible velocities, namely all velocities larger than the linear velocity. To obtain the unique velocity of a front propagating into a metastable state, one has to solve the differential equation in the frame co-moving with the front and find the front shape. Since the differential equation is nonlinear, this is not an easy task. Often, one has to resort to some trial parametric solution and substitute it into the differential equation to calculate the parameter values. As a typical example we consider the reaction term $F(\rho) = r(\rho - \rho_1)(\rho_2 - \rho)(\rho - \rho_3)$, where $\rho_1 < \rho_2 < \rho_3$. This kinetic term has the steady states $\overline{\rho} = \rho_i$, with $i = 1, 2, 3$. The states ρ_1 and ρ_3 are stable, while ρ_2 is unstable. To obtain the front profile and velocity, we need to solve the differential equation

$$D\rho_{zz} + v\rho_z + r(\rho - \rho_1)(\rho_2 - \rho)(\rho - \rho_3) = 0. \tag{4.22}$$

Since the front joins the two stable states and propagates into the metastable state, the boundary conditions are given by

$$\lim_{z\to-\infty} \rho(z) = \rho_3 \quad \text{and} \quad \lim_{z\to+\infty} \rho(z) = \rho_1. \tag{4.23}$$

The derivative ρ_z must vanish at $\rho = \rho_3$ and at $\rho = \rho_1$. A possible candidate for the front solution is $\rho_z = b(\rho - \rho_1)(\rho - \rho_3)$, where b is a constant to be determined. Substituting this solution into (4.22), we obtain a cubic polynomial in ρ. Setting the coefficients to 0 provides a system of four algebraic equations. The equation for the coefficient of ρ^3 yields $b = \sqrt{r/2D}$. With this value, the equations for the coefficient of ρ^2 and ρ^0 are satisfied, and only one equation remains to be solved. The equation for the coefficient of ρ provides the relation for the velocity:

$$v = \sqrt{\frac{rD}{2}} \left(\rho_1 - 2\rho_2 + \rho_3\right). \tag{4.24}$$

Finally, we calculate the front profile by integrating

$$\rho_z = \sqrt{r/2D}(\rho - \rho_1)(\rho - \rho_3) \tag{4.25}$$

and imposing the boundary conditions. The result is

$$\rho(z) = \frac{\rho_3 + K\rho_1 \mathrm{e}^{\sqrt{r/2D}(\rho_3 - \rho_1)z}}{1 + K\mathrm{e}^{\sqrt{r/2D}(\rho_3 - \rho_1)z}}, \tag{4.26}$$

where K is an arbitrary constant that can be determined, e.g, by imposing a value for $\rho(z = 0)$. Equation (4.24) implies that $v > 0$ if $\rho_2 < (\rho_1 + \rho_3)/2$, and it is negative otherwise. This means that we can change the direction of front propagation for fixed values of ρ_1 and ρ_3 by varying the value of ρ_2. Changing ρ_2 affects the relative stability of the stable states ρ_1 and ρ_3, i.e., which one is the stable and the metastable state, and thus the direction of front motion. This can be easily understood by invoking the dynamical picture introduced in Sect. 4.1. The potential difference between states ρ_1 and ρ_3 is given by

$$\Delta V = V(\rho_3) - V(\rho_1) = \int_{\rho_1}^{\rho_3} F(\rho)\mathrm{d}\rho = \frac{(\rho_3 - \rho_1)^3}{12} \left(\rho_1 - 2\rho_2 + \rho_3\right). \tag{4.27}$$

If $\rho_2 < (\rho_1 + \rho_3)/2$, $V(\rho_3) > V(\rho_1)$, and ρ_3 is stable, while ρ_1 is metastable. In this case, the front travels to the right, $v > 0$, by invading ρ_1 (remember that $\rho_1 < \rho_3$). Otherwise, if $\rho_2 > (\rho_1 + \rho_3)/2$, $V(\rho_1) > V(\rho_3)$, and ρ_1 is stable, while ρ_3 is metastable; the front propagates to the left. This is depicted in Fig. 4.3. The sign of the front velocity, i.e., the direction of propagation, can be determined for a general kinetic term $F(\rho)$. We multiply (4.2) by ρ_z and integrate over z to obtain

$$\int_{-\infty}^{\infty} \rho_{zz}\rho_z \mathrm{d}z + v\int_{-\infty}^{\infty} \rho_z^2 \mathrm{d}z + \int_{-\infty}^{\infty} F(\rho)\rho_z \mathrm{d}z = 0. \tag{4.28}$$

The first integral is

$$\int_{-\infty}^{\infty} \rho_{zz}\rho_z \mathrm{d}z = \frac{1}{2}\left[\rho_z^2\right]_{-\infty}^{+\infty} = 0, \tag{4.29}$$

and the third one is

$$\int_{-\infty}^{\infty} F(\rho)\rho_z \mathrm{d}z = \int_{\rho_1}^{\rho_3} F(\rho)\mathrm{d}\rho, \tag{4.30}$$

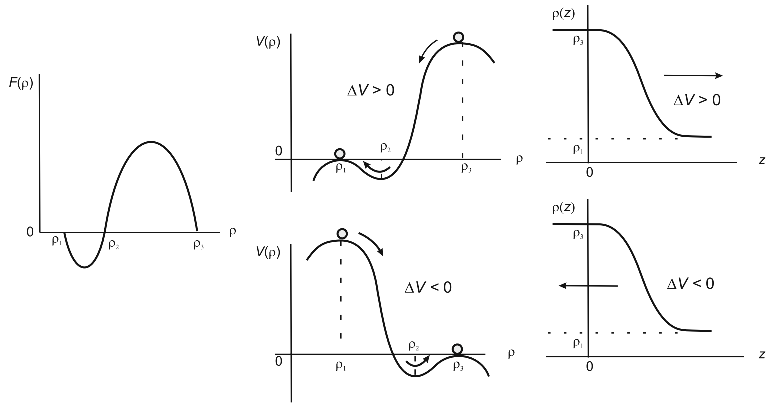

Fig. 4.3 The potential difference between the stable steady states changes their relative stability and changes the direction of front propagation

so that

$$v = \frac{\int_{\rho_1}^{\rho_3} F(\rho)\mathrm{d}\rho}{\int_{-\infty}^{\infty} \rho_z^2 \mathrm{d}z} \tag{4.31}$$

and

$$\mathrm{sgn}(v) = \mathrm{sgn}\left(\int_{\rho_1}^{\rho_3} F(\rho)\mathrm{d}\rho\right). \tag{4.32}$$

For the case (4.22), $\mathrm{sgn}(v) = \mathrm{sgn}\left(\rho_1 - 2\rho_2 + \rho_3\right)$, in agreement with (4.24).

4.2 Front Velocity Selection

The fact that an infinity of front velocities occurs for pulled fronts gives rise to the problem of velocity selection. In this section we present two methods to tackle this problem. The first method employs the Hamilton–Jacobi theory to analyze the dynamics of the front position. It is equivalent to the marginal stability analysis (MSA) [448] and applies only to pulled fronts propagating into unstable states. However, in contrast to the MSA method, the Hamilton–Jacobi approach can also deal with pulled fronts propagating in heterogeneous media, see Chap. 6. The second method is a variational principle that works both for pulled and pushed fronts propagating into unstable states as well as for those propagating into metastable states. This principle can deal with the problem of velocity selection, if it is possible to find the proper trial function. Otherwise, it provides only lower and upper bounds for the front velocity.

4.2.1 Hamilton–Jacobi Formalism

4.2.1.1 Hyperbolic Scaling and Hamilton–Jacobi Equation for the Front Position

This method consists in finding the Hamilton–Jacobi equation for an RD equation with a KPP reaction term and was originally introduced by Freidlin [140]. The first step consists in performing the hyperbolic scaling on the RD equation (2.3):

$$x \to \frac{x}{\varepsilon} \quad \text{and} \quad t \to \frac{t}{\varepsilon}, \quad \varepsilon \ll 1. \tag{4.33}$$

The second step consists in analyzing the behavior of solutions of (2.3) for large times, of order ε^{-1}, and determine whether or not a front exists in the limit $t \to \infty$ ($\varepsilon \to 0$). We expect that after the hyperbolic scaling the new field $\rho^{\varepsilon}(x,t) = \rho(x/\varepsilon, t/\varepsilon)$ takes only two values, 0 and 1, as $\varepsilon \to 0$, which means that the solution of (2.3) converges to the indicator function of the set whose boundary can be considered as the position of a moving front that separates the stable and unstable states. In fact any initial condition with compact support will ensure a front propagating with the minimal velocity. After the hyperbolic scaling, (2.3) reads

$$\varepsilon \frac{\partial \rho^{\varepsilon}}{\partial t} = D\varepsilon^2 \frac{\partial^2 \rho^{\varepsilon}}{\partial x^2} + rF(\rho^{\varepsilon}). \tag{4.34}$$

Since $\rho^{\varepsilon}(x,t) \geq 0$, we can make use of the transformation

$$\rho^{\varepsilon}(x,t) = \exp\left[-G^{\varepsilon}(x,t)/\varepsilon\right], \tag{4.35}$$

where $G^{\varepsilon}(x,t) \geq 0$. The new function $G^{\varepsilon}(x,t)$ determines the location of the front in the limit $\varepsilon \to 0$. If $F(\rho) = \rho(1-\rho)$, straightforward calculations show that $G^{\varepsilon}(x,t)$ obeys the equation

$$-\frac{\partial G^{\varepsilon}}{\partial t} = -D\varepsilon \frac{\partial^2 G^{\varepsilon}}{\partial x^2} + D\left(\frac{\partial G^{\varepsilon}}{\partial x}\right)^2 + r\left[1 - \mathrm{e}^{-G^{\varepsilon}(x,t)/\varepsilon}\right]. \tag{4.36}$$

Since $\exp\left[-G^{\varepsilon}/\varepsilon\right] \to 0$ as $\varepsilon \to 0$ for $G^{\varepsilon} > 0$, we conclude that the limiting function $G(x,t) = \lim_{\varepsilon\to 0} G^{\varepsilon}(x,t)$ obeys the classical Hamilton–Jacobi equation

$$-\frac{\partial G}{\partial t} = D\left(\frac{\partial G}{\partial x}\right)^2 + r. \tag{4.37}$$

Indeed, we obtain the classical Hamiltonian, $H = Dp^2 + r$, if we define

$$H = -\frac{\partial G}{\partial t} \quad \text{and} \quad p = \frac{\partial G}{\partial x}. \tag{4.38}$$

4.2.1.2 Propagation Velocity

The hyperbolic scaling (4.33) and the transformation (4.35) of the field allows us to obtain, in the asymptotic limit $\varepsilon \to 0$, a Hamilton–Jacobi equation for any given reaction–transport equation. In this chapter we focus only on RD equations, but in Chap. 5 we deal with other models. Regardless of the specific form of the Hamilton–Jacobi equation, its solution can be written as

$$G(x,t) = \inf_{x(0)=0,x(t)=x} \left[\int_0^t L(x,s)\mathrm{d}s \right], \tag{4.39}$$

where

$$L(x,s) = p(s)\frac{\mathrm{d}x(s)}{\mathrm{d}s} - H(x,s) \tag{4.40}$$

is the Lagrangian and s the temporal coordinate. $x(s)$ and $p(s)$ satisfy the Hamilton equations

$$\frac{\mathrm{d}x}{\mathrm{d}s} = \frac{\partial H}{\partial p}, \quad \frac{\mathrm{d}p}{\mathrm{d}s} = -\frac{\partial H}{\partial x}, \tag{4.41}$$

with the conditions $x(0) = 0$, $x(t) = x$. The location of the front position is determined by the equation $G(x(t),t) = 0$, and the propagation velocity can be found as follows. Differentiating $G(x(t),t) = 0$ and taking into account $v = \mathrm{d}x/\mathrm{d}t$, one writes

$$\frac{\partial G}{\partial t} + v\frac{\partial G}{\partial x} = 0 \tag{4.42}$$

or using (4.38)

$$v = \frac{H}{p}. \tag{4.43}$$

If the reaction–transport equations are homogeneous, i.e., there is no explicit dependence on time or space coordinates, then the Hamilton–Jacobi equation is of the form $H = H(p)$. (The case with spatial or temporal heterogeneities is dealt with in Chap. 6.) The Hamilton equations (4.41) imply that p is constant and that

$$x(s) = \frac{\partial H}{\partial p}s, \quad \frac{\partial H}{\partial p} = \frac{x}{t}, \tag{4.44}$$

where we have made use of the boundary conditions. From (4.39) and (4.44)

$$G(x,t) = px - H(p)t, \tag{4.45}$$

and the front position evolves according to $x/t = H/p$, which combined with the second equation in (4.44) and (4.43) yields a closed system of algebraic equation to calculate the front velocity,

$$v = \frac{\partial H}{\partial p}, \quad \text{and} \quad \frac{\partial H}{\partial p} = \frac{H}{p}. \tag{4.46}$$

This system of equations can be summarized in the single equation

$$v = \min_{p>0} \left[\frac{H(p)}{p} \right]. \tag{4.47}$$

In the case of the RD equation,

$$v = \min_{p>0} \left[\frac{Dp^2 + r}{p} \right] = 2\sqrt{rD}, \tag{4.48}$$

which is known as the Fisher velocity.

4.2.2 Variational Characterization

We follow here the derivation by Benguria and Depassier [34, 35]. The starting point for the variational principle is the ordinary differential equation for the RD equation in the frame comoving with the front (4.2). Without loss of generality, we assume that the front connects the states $\rho = 0$ and $\rho = 1$, i.e., $\lim_{z\to\infty} \rho = 0$ and $\lim_{z\to-\infty} \rho = 1$. Since the front is monotonic, we define $q(\rho) = -\rho_z > 0$. Monotonic fronts are solutions of

$$Dq(\rho)\frac{\mathrm{d}q}{\mathrm{d}\rho} - vq(\rho) + F(\rho) = 0, \tag{4.49}$$

with

$$q(0) = 0, \quad q(1) = 0, \tag{4.50}$$

and $q > 0$ in (0, 1).

Let $g(\rho)$ be any positive function on (0, 1), such that $h = -\mathrm{d}g/\mathrm{d}\rho > 0$. Multiplying (4.49) by g/q and integrating with respect to ρ, we obtain

$$\int_0^1 \left(Dhq + \frac{F(\rho)}{q} g \right) \mathrm{d}\rho = v \int_0^1 g\mathrm{d}\rho, \tag{4.51}$$

where the first term is obtained after integration by parts. For fixed ρ, the functional

$$\Phi[q] \equiv Dhq + \frac{F(\rho)}{q} g \tag{4.52}$$

has a minimum at $q_{\min} = \sqrt{Fg/(Dh)}$, since v, q, g, and h are positive. Consequently, $\Phi[q] \geq \Phi[q_{\min}] = 2\sqrt{DFgh}$ and

$$\int_0^1 \Phi[q] \mathrm{d}\rho = v \int_0^1 g \mathrm{d}\rho \geq 2\sqrt{D} \int_0^1 \sqrt{Fgh} \mathrm{d}\rho, \tag{4.53}$$

that is,

$$v \geq 2\sqrt{D} \frac{\int_0^1 \sqrt{Fgh} \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho}. \tag{4.54}$$

This lower bound for the front velocity is valid for any $F(\rho) > 0$ on (0,1) and $F(0) = F(1) = 0$, i.e., for a front propagating into unstable states (reaction terms of Case A) [34]. To show that (4.54) represents indeed a variational principle, we must establish that there exists a function, namely $\breve{g}$, for which the equality holds in (4.54). Equality holds if $\breve{g}$ satisfies $hq = F\breve{g}/(Dq)$, i.e.,

$$-\frac{\mathrm{d}(\ln \breve{g})}{\mathrm{d}\rho} = \frac{v}{Dq} - \frac{\mathrm{d}(\ln q)}{\mathrm{d}\rho}, \tag{4.55}$$

where we have made use of (4.49). This equation can be integrated to yield

$$\breve{g}(\rho) = q(\rho) \exp\left(\int_\rho^{\rho_0} \frac{v}{Dq} \mathrm{d}\rho \right) \tag{4.56}$$

for some fixed ρ_0, $0 < \rho_0 < 1$. Obviously, $\breve{g}(\rho)$ is a continuous, positive, and decreasing function on (0,1) and $\breve{g}(1) = 0$. However, for $\rho \to 0$, a singularity occurs that needs to be handled carefully. We must ensure that the integrals in (4.54) exist for this value. We linearize (4.2) near $\rho = 0$ and find that if $\rho \sim \exp(-\lambda z)$ then $q \sim \lambda_+ \rho$. Here $\lambda_+ = \left[v + \sqrt{v^2 - 4DF'(0)} \right] / 2D$ is the largest root of the characteristic equation for λ. From (4.56)

$$\sqrt{F\breve{g}h} \sim \breve{g}(\rho) \sim \rho^{1 - v/(\lambda_+ D)} \text{ near } \rho = 0. \tag{4.57}$$

Therefore, if $v > 2\sqrt{DF'(0)}$, we have $\int_0^1 g \mathrm{d}\rho < \infty$ and $\int_0^1 \sqrt{Fgh} \mathrm{d}\rho < \infty$. In summary, we have proven that there exists a positive, continuous, and monotonically decreasing function g, for which the integrals in (4.54) exist and which maximizes the lower bound in (4.54) in such a way that the equality holds. In summary,

$$v = \max_g \left(2\sqrt{D} \frac{\int_0^1 \sqrt{Fgh} \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho} \right), \tag{4.58}$$

if $v > 2\sqrt{DF'(0)}$ which is a lower bound for the front velocity. We can obtain from (4.58) also the upper bound derived by Aronson and Weinberger [18]:

$$v = \max_g \left(2\sqrt{D} \frac{\int_0^1 \sqrt{Fgh} \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho} \right) = \max_g \left(2\sqrt{D} \frac{\int_0^1 g\sqrt{Fh/g} \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho} \right)$$
$$\leq 2\sqrt{D} \max_g \sqrt{\frac{\int_0^1 Fh \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho}}, \tag{4.59}$$

where the inequality follows from Jensen's inequality. Since $h > 0$, we have

$$\frac{\int_0^1 Fh \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho} = \frac{\int_0^1 (F/\rho) h\rho \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho} \leq \frac{\int_0^1 h\rho \mathrm{d}\rho}{\int_0^1 g \mathrm{d}\rho} \sup_\rho \left(\frac{F}{\rho} \right) = \sup_\rho \left(\frac{F}{\rho} \right). \tag{4.60}$$

We have used $\int_0^1 h\rho \mathrm{d}\rho = \int_0^1 g \mathrm{d}\rho$, which follows from integration by parts. Finally, we obtain

$$2\sqrt{DF'(0)} < v \leq 2\sqrt{D} \sqrt{\sup_\rho \left(\frac{F}{\rho} \right)}, \tag{4.61}$$

which is the result given in (4.12).

Note that the variational characterization given in (4.58) only holds if $F > 0$ on (0,1) and for fronts propagating into unstable states. To derive a variational result valid if $F < 0$ for some values of ρ, we need to extend these results [35]. To do so, we multiply (4.49) by g. Integrating between $\rho = 0$ and $\rho = 1$, we obtain after integration by parts

$$\int_0^1 F(\rho) g \mathrm{d}\rho = v \int_0^1 qg \mathrm{d}\rho - \frac{1}{2} D \int_0^1 hq^2 \mathrm{d}\rho. \tag{4.62}$$

For fixed ρ, the functional

$$\Phi[q] \equiv vqg - \frac{1}{2} Dhq^2 \tag{4.63}$$

has a maximum at $q_{\max} = vg/(Dh)$, since v, q, g, and h are positive. Therefore $\Phi[q] \leq \Phi[q_{\max}] = v^2 g^2/(2Dh)$ for any value of ρ. It follows that

$$v^2 \geq 2D \frac{\int_0^1 F g \mathrm{d}\rho}{\int_0^1 (g^2/h) \mathrm{d}\rho}, \tag{4.64}$$

which holds for any $F(\rho)$ for which a monotonic front exists. The equality in (4.64) holds if $\breve{g}$ satisfies

$$-\frac{\mathrm{d}(\ln \breve{g})}{\mathrm{d}\rho} = \frac{v}{Dq}, \tag{4.65}$$

which can be integrated to yield

$$\breve{g}(\rho) = \exp\left(\int_\rho^{\rho_0} \frac{v}{Dq} \mathrm{d}\rho\right). \tag{4.66}$$

Obviously, $\breve{g}(\rho)$ is again a continuous, positive, and decreasing function on (0,1) with $\breve{g}(1) = 0$. Near $\rho = 0$, $\breve{g}$ diverges. We linearize (4.2) to find from (4.66)

$$\breve{g}(\rho) \sim \rho^{-v/(\lambda_+ D)} \text{ near } \rho = 0, \tag{4.67}$$

and $f\breve{g} \sim (\breve{g})^2/h \sim \rho^{1-v/(\lambda_+ D)}$. The integrals in (4.64) exist if $\lambda_+ D/v > 1/2$. This condition is always satisfied if $F'(0) \leq 0$, i.e., for Case B (front propagating into metastable states). However, it is also satisfied for Case A (fronts propagating into unstable states) provided that $v > 2\sqrt{DF'(0)}$. The asymptotic front velocity is given for both cases A and B by

$$v^2 = \max_g \left[2D \frac{\int_0^1 F g \mathrm{d}\rho}{\int_0^1 (g^2/h) \mathrm{d}\rho}\right], \tag{4.68}$$

where the maximum is taken over all positive, decreasing trial functions on (0,1) for which the integrals exist.

We illustrate the power of the variational characterization (4.68) by solving some examples for cases A and B. To do so, we will consider the trial function

$$g(\rho) = \rho^{-\mu}(1-\rho)^{\mu} \quad \text{with} \quad \mu > 0. \tag{4.69}$$

We maximize over all possible values of μ for which the integrals in the variational formula exist:

$$v^2 = \max_{0<\mu\leq 2} 2D \left[\frac{\mu\Gamma(4)}{\Gamma(2-\mu)\Gamma(2+\mu)} \int_0^1 F(\rho)\rho^{-\mu}(1-\rho)^{\mu} \mathrm{d}\rho\right]. \tag{4.70}$$

KPP reaction term. With $F(\rho) = \rho(1-\rho)$ (4.70) yields

$$v^2 = 2D \max_{0<\mu\leq 2} \mu, \tag{4.71}$$

i.e., $v = 2\sqrt{D}$.

Pulled–Pushed transition. The variational characterization can account for the pulled–pushed transition for fronts propagating into unstable states. We consider the Ben-Jacob case [37], where $F(\rho) = \rho(1-\rho)(1+\alpha\rho)$ with $\alpha > 0$. Equation (4.70) yields

$$v^2 = \max_{0<\mu\leq 2} 2D\mu \left[1 + \frac{\alpha}{4}(2-\mu)\right]. \tag{4.72}$$

The maximum must be evaluated carefully for this case. For $\alpha \leq 2$, the maximum occurs at $\mu = 2$ and for $\alpha \geq 2$ at $\mu = (\alpha+2)/\alpha$,

$$v = \begin{cases} 2\sqrt{D}, & \alpha \leq 2, \\ \sqrt{D/2}\left(\sqrt{\alpha} + 2/\sqrt{\alpha}\right), & \alpha \geq 2, \end{cases} \tag{4.73}$$

which coincides with Ben-Jacob's result.

Cubic reaction term. We deal again with the case considered in (4.22) for a front propagating into a metastable state, i.e., connecting ρ_1 and ρ_3. To apply (4.70), where it is assumed that the front connects 0 and 1, we rescale (4.22) by defining the new field $u = (\rho - \rho_1)/(\rho_3 - \rho_1)$. Equation (4.22) then reads

$$Du_{zz} + vu_z + rau(1-u)(u-b), \tag{4.74}$$

where

$$a \equiv (\rho_3 - \rho_1)^2 \quad \text{and} \quad b \equiv \frac{\rho_2 - \rho_1}{\rho_3 - \rho_1} > 0. \tag{4.75}$$

Substitute the reaction term $F(u) = rau(1-u)(u-b)$ into (4.70). Then

$$v^2 = \max_{0<\mu\leq 2} D\mu ar \left[1 - \frac{\mu}{2} - 2b\right]. \tag{4.76}$$

In this case, the maximum occurs at $\mu = 1 - 2b$,

$$v = \sqrt{\frac{raD}{2}}(1-2b) = \sqrt{r\frac{D}{2}}(\rho_3 - 2\rho_2 + \rho_1), \tag{4.77}$$

which is exactly the same result as in (4.24). Furthermore, we can also obtain the front profile from the variational characterization. The selected front is the one that satisfies the equality in (4.64), and the front profile is given by $q = vg/(Dh)$:

$$-\frac{\mathrm{d}u}{\mathrm{d}z} = \frac{vg}{Dh} = \sqrt{\frac{r}{2D}}(\rho_3 - \rho_1)u(1-u). \tag{4.78}$$

Since $u = (\rho - \rho_1)/(\rho_3 - \rho_1)$, the above equation turns into

$$\frac{\mathrm{d}\rho}{\mathrm{d}z} = \sqrt{\frac{r}{2D}}(\rho - \rho_1)(\rho - \rho_3), \tag{4.79}$$

which coincides with (4.25) for the front profile.

4.3 Effect of Low Concentrations

The sensitivity of fronts to the dynamics of small perturbations about the unstable or metastable states has been studied by Brunet and Derrida [61] for pulled fronts and Kessler et al. [227] for pulled and pushed fronts. The mean-field description of reacting and diffusing systems ceases to be valid for low values of the particle density ρ, values that correspond to less than one particle. This fact can be incorporated into the RD equation by introducing a cutoff for the reaction term. Such a cutoff strongly affects the front velocity. Throughout this section we consider for simplicity that space and time have been rescaled such that $D = r = 1$.

4.3.1 Effect on Pulled Fronts

The starting point of Brunet and Derrida's approach is to replace the kinetic term in the FKPP equation by $F(\rho) = \theta(\rho - \epsilon)\rho(1-\rho)$. Here $\theta(\cdot)$ denotes the Heaviside function, and $\epsilon = 1/N$ is the cutoff, where N is the average number of particles in the state $\rho = 1$. In the frame comoving with the front, the RD equation

$$\rho_{zz} + v_\epsilon \rho_z + \theta(\rho - \epsilon)\rho(1-\rho) = 0 \tag{4.80}$$

can be divided into three regions. In region II, $\epsilon < \rho \ll 1$, the nonlinear terms in the reaction function can be ignored. In region III, $\rho < \epsilon$, the kinetic term vanishes. In region I, ρ is not small compared to 1, and one has to consider the full nonlinear equation without cutoff. These considerations lead to the system of equations:

$$\rho_{zz} + v_\epsilon \rho_z + \rho(1-\rho) = 0, \quad \text{in region I,} \tag{4.81a}$$

$$\rho_{zz} + v_\epsilon \rho_z + \rho \simeq 0, \quad \text{in region II,} \tag{4.81b}$$

$$\rho_{zz} + v_\epsilon \rho_z = 0, \quad \text{in region III.} \tag{4.81c}$$

At the boundary between regions I and II and the boundary between II and III, the particle density ρ, as well as its comoving derivative ρ_z, must be continuous. Since $\epsilon \ll 1$, the solutions of (4.81) are given to leading order by

$$\rho(z) = \epsilon e^{-v_\epsilon(z-z_0)}, \quad \text{in region III, and} \tag{4.82a}$$

$$\rho(z) \sim \sin\left(\frac{\pi z}{|\ln \epsilon|}\right) e^{-z}, \quad \text{in region II,} \tag{4.82b}$$

where $z_0 \simeq |\ln \epsilon|$ marks the boundary between regions II and III. The continuity conditions at the boundary between both regions lead to

$$v_\epsilon \simeq 2 - \frac{\pi^2}{(\ln \epsilon)^2}. \tag{4.83}$$

The velocity converges to 2 as $(\ln \epsilon)^{-2}$ or $(\ln N)^{-2}$.

4.3.2 Effect on Pushed Fronts

For fronts propagating into metastable states and pushed fronts propagating into unstable states, Kessler et al. [227] showed that the velocity shift introduced by the cutoff depends on a power of ϵ. Consider a RD equation with a cutoff around the state $\rho = 0$, where the linear part of the growth term is ρ. In the nonreacting region III, i.e., $z > z_0$, and the region corresponding to large z with $z < z_0$, the solutions of the RD equation are

$$\rho(z) = \epsilon e^{-v_\epsilon(z-z_0)}, \quad \text{for } z > z_0, \tag{4.84a}$$

$$\rho(z) = A_1 e^{-\lambda_+ z} + \delta v A_2 e^{-\lambda_- z}, \quad \text{for large } z \text{ with } z < z_0. \tag{4.84b}$$

Here

$$\lambda_\pm = \frac{v_0 \pm \sqrt{v_0^2 - 4}}{2}, \tag{4.85}$$

and v_0 is the front velocity in the absence of a cutoff, i.e., $v_\epsilon = v_0 + \delta v$. The integration constants A_1 and A_2 do not depend on ϵ and can be obtained by matching the solutions at the boundary, treating δv as a small parameter. At $z = z_0$, the two terms in (4.84b) must be of the same order, $e^{-\lambda_+ z_0} \sim \delta v e^{-\lambda_- z_0}$, or $\delta v \sim e^{z_0(\lambda_- - \lambda_+)}$. The matching condition implies that $e^{-\lambda_+ z_0} \sim \epsilon$, or $z_0 \sim -\ln \epsilon / \lambda_+$, and

$$\delta v \sim \epsilon^{1-\frac{\lambda_-}{\lambda_+}} = \epsilon^{1+\frac{\sqrt{1-4/v_0^2}-1}{\sqrt{1-4/v_0^2}+1}}. \tag{4.86}$$

We consider first an example of a pushed front propagating into an unstable state, namely Ben-Jacob's case with a cutoff, $F(\rho) = \theta(\rho - \epsilon)\rho(1 - \rho)(1 + \alpha\rho)$. A pushed front occurs for $\alpha > 2$ and $v_0 = (\sqrt{\alpha} + 2/\sqrt{\alpha})/\sqrt{2}$, see (4.14). In this case, $\delta v \sim \epsilon^{(\alpha-2)/\alpha}$, i.e., a sublinear dependence of the shift in the front velocity on the cutoff.

We consider next a front propagating into a metastable state for the Nagumo equation, $F(\rho) = \theta(\rho - \epsilon)\rho(1 - \rho)(\rho - a)$. The front velocity in the absence of a cutoff is $v_0 = 1/\sqrt{2} - a\sqrt{2}$. Equation (4.86) yields $\delta v \sim \epsilon^{1+2a}$. Exact analytical results for the front solutions can be obtained if the reaction term $F(\rho)$ with a cutoff is replaced by a piecewise linear approximation. The dependence of the velocity shift on the cutoff displays good agreement with the results by Brunet and Derrida and Kessler et al. [495].

4.3.3 Variational Principles and the Cutoff Problem

Recent studies have applied improved variational principles to deal with the velocity shift due to a cutoff in the reaction term, both for fronts propagating into unstable and metastable states [284, 36]. They confirm the results by Brunet and Derrida and improve the results by Kessler et al. The variational principle given in (4.68) implies that for any admissible trial function a lower bound for the velocity can be found by (4.64). The trial function for which equality in (4.64) holds diverges at $\rho = 0$, and it is convenient to consider trial functions that in addition to the requirements $g > 0$ and $g' < 0$ also satisfy $g(0) \to \infty$. Such trial functions allow us to obtain accurate lower bounds for the front velocity. We perform a change of variables $\rho = \rho(s)$, where $s = 1/g$, and consider s as the independent variable in (4.68). With this change of variables, the variational principle reads

$$v^2 = \max_{\rho(s)} 2 \frac{V(1)/s_0 + \int_0^{s_0} \left(V[\rho(s)]/s^2 \right) \mathrm{d}s}{\int_0^{s_0} (\mathrm{d}\rho/\mathrm{d}s)^2 \, \mathrm{d}s}. \tag{4.87}$$

Here $s_0 = 1/g(\rho = 1)$, $V(\rho) = \int_0^{\rho} F(u)\mathrm{d}u$, and the maximum is taken over positive increasing functions $\rho(s)$, such that $\rho(0) = 0$ and for which the integrals in (4.87) converge. Consider the reaction term $F(\rho) = \theta(\rho - \epsilon)\rho(1 - \rho^2)$ and the trial function

$$\rho(s) = \begin{cases} s, & \text{if } 0 \le s \le \epsilon, \\ \sqrt{\epsilon s} \sqrt{1 + \frac{(\ln \epsilon)^2}{4\phi^2}} \cos\left[\frac{\phi}{|\ln \epsilon|} \ln(s/\epsilon) - \phi \right], & \text{if } \epsilon \le s \le \epsilon^{-1}, \end{cases} \tag{4.88}$$

where ϕ is the solution of the equation $\phi \tan \phi - |\ln \epsilon| /2 = 0$. Substituting this trial function into (4.87), we find the lower bound

$$v^2 \ge 4 \left(1 - \frac{\pi^2}{|\ln \epsilon|^2} + \cdots \right) \tag{4.89}$$

after expanding for small ϵ. For pushed fronts, the existence of a variational principle allows one to use the Feynman–Hellman theorem to calculate the dependence of the velocity on parameters of the reaction term [36]. If the reaction term is of the form $F(\rho) = F(\rho, \alpha)$ then

$$\frac{\partial v^2}{\partial \alpha} = 2\frac{\int_0^1 \frac{\partial F(\rho,\alpha)}{\partial \alpha}\breve{g}(\rho,\alpha)\mathrm{d}\rho}{\int_0^1 \left(-\breve{g}^2/\breve{g}'\right)\mathrm{d}\rho}, \tag{4.90}$$

where $\breve{g}$ is the trial function, unique up to a multiplicative constant, that produces the maximum in (4.68) for the given parameter α. Note that the Feynman–Hellman theorem only holds, if the maximum is actually realized, which is not the case for pulled fronts. Consider the reaction term $F(\rho) = \theta(\rho - \epsilon) f(\rho)$ and $\alpha \equiv \epsilon$. The Feynman–Hellman theorem (4.90) implies that

$$\frac{\partial v^2}{\partial \epsilon} = 2\frac{\int_0^1 \breve{g}(\rho,\epsilon)\frac{\partial}{\partial \epsilon}\left[\theta(\rho-\epsilon)f(\rho)\right]\mathrm{d}\rho}{\int_0^1 \left(-\breve{g}^2/\breve{g}'\right)\mathrm{d}\rho} = -2\frac{\breve{g}(\epsilon,\epsilon)f(\epsilon)}{\int_0^1 \left(-\breve{g}^2/\breve{g}'\right)\mathrm{d}\rho}. \tag{4.91}$$

For small ϵ, the leading order of the trial function $\breve{g}(\rho,\epsilon)$ is $\breve{g}(\rho,0) \equiv \breve{g}_0(\rho)$, which is exactly the optimizing function for the case without a cutoff. On the other hand, for small ϵ we can write $v(\epsilon) = v_0 + \epsilon\,(\partial v/\partial \epsilon)_{\epsilon=0} + \cdots$, so that

$$\delta v = \epsilon \frac{\partial v}{\partial \epsilon}\bigg|_{\epsilon=0} = -\frac{1}{v_0 \int_0^1 \left(-\breve{g}_0^2/\breve{g}_0'\right)\mathrm{d}\rho}\epsilon f(\epsilon)\breve{g}_0(\epsilon), \tag{4.92}$$

where we have made use of the variational result for the case without cutoff:

$$v_0^2 = 2\frac{\int_0^1 f(\rho)\breve{g}_0(\rho)\mathrm{d}\rho}{\int_0^1 \left(-\breve{g}_0^2/\breve{g}_0'\right)\mathrm{d}\rho}. \tag{4.93}$$

From (4.67) we know that $\breve{g}_0(\rho) \sim \rho^{-v_0/\lambda_+}$ near $\rho = 0$, with

$$\lambda_+ = \frac{1}{2}\left[v_0 + \sqrt{v_0^2 - 4f'(0)}\right], \tag{4.94}$$

and $\breve{g}_0(\epsilon) \sim \epsilon^{-v_0/\lambda_+}$. Since the denominator in (4.92) is a positive constant and does not depend on ϵ, we conclude that

$$\delta v \sim \begin{cases} -f(\epsilon), & \text{if } f'(0) = 0, \\ -f'(0)\epsilon^{2-v_0/\lambda_+}, & \text{if } f'(0) \neq 0. \end{cases} \tag{4.95}$$

These results are in agreement with the previous results obtained from a different variational principle and also with the results obtained by Kessler et al. The dependence of the second result is exactly that given in (4.86).

4.4 Effect of External Noise

In this section we explore the systematic effect of an external noise on the front velocity. Consider a reaction term $F(\rho, \alpha)$ that depends not only on the density but also on a parameter α that fluctuates. Assuming small fluctuations around its mean value, we can write $\alpha(x, t) = \alpha_m - \epsilon^{1/2}\eta(x, t)$, where α_m is the mean value, ϵ is a small parameter governing the noise amplitude, and $\eta(x, t)$ is a Gaussian noise with zero mean and correlation given by

$$\left\langle \eta(x, t)\eta(x', t') \right\rangle = 2C(x - x')\delta(t - t'), \tag{4.96}$$

where $\delta(\cdot)$ is the Dirac delta-function and $\langle \cdot \rangle$ denotes averaging. The role of spatiotemporal structured noise has been discussed in [377]. For simplicity, we consider here noise that is white in time and correlated in space [376]. This is an excellent approximation if the time scale of the noise is much shorter than the characteristic time of the kinetics. We assume that the fluctuations have a small amplitude, $F(\rho, \alpha) = F(\rho, \alpha_m) - \frac{\partial F}{\partial \alpha}\epsilon^{1/2}\eta(x, t) + O(\epsilon)$. Then the RD equation can be written as the following stochastic partial differential equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} + f(\rho) + \epsilon^{1/2} g(\rho)\eta(x, t), \tag{4.97}$$

where $f(\rho) = F(\rho, \alpha_m)$ and $g(\rho) = -\frac{\partial F}{\partial \alpha}(\rho, \alpha_m)$. The noise appears in the RD equation (4.97) in a multiplicative way. An additive noise source can also be included to account for fluctuations due to internal noise. Additive noise does not modify the front velocity for the invasion of either metastable or unstable states, and the front itself exists only during a short transient period. We consider here only the case of a multiplicative noise. The effects on front propagation are twofold: First, multiplicative noise produces a random meandering of the front position with respect to its mean position [17, 16]. Second, multiplicative noise induces a shift in the mean front velocity. We focus on the second effect; the problem reduces to an analogous deterministic problem with renormalized coefficients.

A crucial feature of the multiplicative noise case is that the noise term in (4.97) has a nonzero mean value. Using Novikov's theorem [324] for Gaussian noise in the Stratonovich interpretation, we find that

$$\epsilon^{1/2} \langle g(\rho)\eta(x, t) \rangle = \epsilon C(0) \left\langle g(\rho)g'(\rho) \right\rangle . \tag{4.98}$$

According to this result, (4.97) can be rewritten as

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} + h(\rho) + \epsilon^{1/2} R(\rho, x, t), \tag{4.99}$$

where

$$h(\rho) \equiv f(\rho) + \epsilon C(0) g(\rho) g'(\rho) \tag{4.100}$$

and

$$R(\rho, x, t) \equiv g(\rho)\eta(x, t) - \epsilon^{1/2} C(0) g(\rho) g'(\rho). \tag{4.101}$$

The stochastic term in (4.99) has zero mean, $\langle R(\rho, x, t)\rangle = 0$, and correlation

$$\left\langle R(\rho, x, t) R(\rho, x', t')\right\rangle = \left\langle g(\rho(x, t))\eta(x, t) g(\rho(x', t'))\eta(x', t')\right\rangle + O(\epsilon^{1/2}). \tag{4.102}$$

This rearrangement allows us to distinguish explicitly between the systematic contribution from the noise term and a residual stochastic one. Since the noise is white in time, the average of the noise term has no explicit time dependence. Writing $\rho(x, t) = \rho_0(x, t) + \delta\rho$, where $\rho_0(x, t) = \langle \rho(x, t)\rangle$ and the perturbative fluctuation is $\delta\rho \sim O(\epsilon^{1/2})$, we obtain to lowest order

$$\frac{\partial \rho_0}{\partial t} = \frac{\partial^2 \rho_0}{\partial x^2} + f(\rho_0) + \epsilon C(0) g(\rho_0) g'(\rho_0), \tag{4.103}$$

which is the RD equation for the mean front profile. The methods developed in Sect. 4.2 allow us to study fronts connecting the steady states of (4.103) and to obtain the mean velocity in terms of the noise intensity $\epsilon(0) \equiv \epsilon C(0)$.

To illustrate our approach, we consider the Ginzburg–Landau reaction term $F(\rho) = \rho(1 - \rho)(\alpha + \rho)$, where $\alpha \rightarrow \alpha_m - \epsilon^{1/2}\eta(x, t)$. Then $f(\rho_0) = \rho_0(1 - \rho_0)(\alpha_m + \rho_0)$ and $g(\rho_0) = -\rho_0(1 - \rho_0)$. In the absence of noise, the velocity of the front propagating into the unstable state 0 is given by

$$v = \begin{cases} (1 + 2\alpha)/\sqrt{2}, & -1/2 < \alpha < 1/2 \text{ (nonlinear)}, \\ 2\sqrt{\alpha}, & 1/2 \leq \alpha \text{ (linear)}, \end{cases} \tag{4.104}$$

a result that can be obtained directly from (4.70). In the presence of multiplicative noise, the mean front profile is governed by (4.103), which reads in this case

$$\frac{\partial \rho_0}{\partial t} = \frac{\partial^2 \rho_0}{\partial x^2} + \rho_0(1 - \rho_0)(\alpha'_m + \beta\rho_0), \tag{4.105}$$

with $\alpha_m' = \alpha_m + \epsilon(0)$ and $\beta = 1 - 2\epsilon(0)$. Applying the variational formula (4.70) to the RD equation (4.105), we obtain the velocity for the front propagating, in the presence of noise, into the unstable state 0:

$$v = \begin{cases} (1+2\alpha_m)/\sqrt{2[1-2\epsilon(0)]}, & -1/2 \leq \alpha_m < 1/2 - 2\epsilon(0) \text{ (nonlinear)}, \\ 2\sqrt{\alpha_m + \epsilon(0)}, & 1/2 - 2\epsilon(0) \leq \alpha_m < 1 \text{ (linear)}. \end{cases} \tag{4.106}$$

An important condition for propagating fronts to exist is that $\epsilon(0) < 1/2$, otherwise the above result does not hold and the presence of noise can destroy the front formation. This result shows that multiplicative noise, which is white in time, can modify the mean front velocity as well as the transition point from the linear to the nonlinear regime of propagation.

4.5 Effect of Time Delay and Age Structure

The inclusion of age structure in RD equations has its origin in the generalization of population growth models. Age-structured models take explicitly into account that population growth is due only to adult individuals. The oldest such model is described by the McKendrick–von Foerster equation [447]:

$$\frac{\partial \rho(a,t)}{\partial t} + \frac{\partial \rho(a,t)}{\partial a} = -\mu(a,t)\rho(a,t), \tag{4.107}$$

where $\rho(a,t)$ is the age distribution density of the population. Let $\rho(a,t)\mathrm{d}a$ be the density of individuals with an age in the interval $(a, a+\mathrm{d}a)$ at time t. The rate of change of the number of individuals in a given age interval Δa is due to the rate of entry at age a minus the rate of departure at age $a + \mathrm{d}a$ minus the deaths, which yields the balance equation

$$\frac{\partial \rho(a,t)}{\partial t}\Delta a = J(a,t) - J(a+\Delta a, t) - \mu(a,t)\rho(a,t)\Delta a. \tag{4.108}$$

Here $\mu(a,t)$ is the per capita mortality rate for individuals of age a at time t, and $J(a,t)$ is the flux of individuals of age a at time t. Dividing by Δa and taking the limit $\Delta a \to 0$, we obtain the conservation equation for the density of individuals:

$$\frac{\partial \rho(a,t)}{\partial t} + \frac{\partial J(a,t)}{\partial a} = -\mu(a,t)\rho(a,t). \tag{4.109}$$

The flux J is not a flux in space, but rather the "movement" of individuals in age. We assume that it is proportional to the density of individuals and some characteristic velocity of aging, $J(a,t) = \rho(a,t)v(a,t)$. Aging is simply the passage of time $v = \mathrm{d}a/\mathrm{d}t = 1$, and we obtain (4.107). If we also include the flux in the space due to the motion of individuals, then we obtain Metz–Diekman model [295]:

$$\frac{\partial \rho(x,a,t)}{\partial t} + \frac{\partial \rho(x,a,t)}{\partial a} = D\frac{\partial^2 \rho(x,a,t)}{\partial x^2} - \mu(a,t)\rho(x,a,t). \tag{4.110}$$

Almost parallel to McKendrick, Hutchinson [215], a well-known ecologist, proposed a time-delayed version for the logistic growth equation, where the nonlinear term was delayed in time. The diffusive Hutchinson equation, also known as the delayed Fisher equation,

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2} + \rho(x,t)\left[1 - \rho(x,t-\tau)\right], \tag{4.111}$$

has front solutions. When the delay τ is large, the traveling wave solution oscillates around the state $\rho = 1$, which can be driven unstable for still larger τ [482]. A generalization of (4.111) consists in incorporating distributed delays in an ad hoc manner by multiplying the second term on the right-hand side of (4.111) by a kernel $k(\tau)$ and integrating over τ. Many other delayed RD equations have appeared in the ecological literature. A particularly well-known one is the Nicholson's blowflies equation:

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2} - \delta\rho(x,t) + p\rho(x,t-\tau)\mathrm{e}^{-\beta\rho(x,t-\tau)}. \tag{4.112}$$

Under certain conditions, this equation has front solutions. However, as for (4.111), loss of monotonicity occurs as the delay is increased and the front develops a prominent hump [167].

There exists a connection between age-structured and time-delayed RD models [169]. From (4.110) we can obtain an equation for the total mature population density $w(x,t)$. Let $f(a)$ be the probability density function of maturation ages, i.e., $f(a)\mathrm{d}a$ is the probability of maturing between the ages a and $a + \mathrm{d}a$. Then the probability of maturing before age a is $F(a) = \int_0^a f(a')\mathrm{d}a'$. The total density of mature individuals is

$$w(x,t) = \int_0^\infty \mathrm{d}a f(a) \int_a^\infty \rho(x,t,a')\mathrm{d}a' = \int_0^\infty \mathrm{d}a F(a)\rho(x,t,a). \tag{4.113}$$

Differentiating (4.113) with respect to time and using (4.110), we obtain

$$\frac{\partial w}{\partial t} = D\frac{\partial^2 w}{\partial x^2} - \mu w + \int_0^\infty \mathrm{d}a f(a)\rho(x,t,a), \tag{4.114}$$

where the diffusion coefficient D and the death rate μ for immature population are assumed to be constants. The solution of (4.110) is given by

$$\rho(x,t,a) = \frac{\mathrm{e}^{-\mu a}}{2\sqrt{\pi D a}} \int_{-\infty}^{\infty} b\left[w(y,t-a)\right] \mathrm{e}^{-(x-y)^2/4Da} \mathrm{d}y, \tag{4.115}$$

where $\rho(x,t=0,a) \equiv b[w(x,t)]$ is the birth function. Inserting this expression into (4.114), we obtain the equation

$$\frac{\partial w}{\partial t} = D\frac{\partial^2 w}{\partial x^2} - \mu w + \int_0^{\infty} \mathrm{d}a f(a) \frac{\mathrm{e}^{-\mu a}}{2\sqrt{\pi D a}} \int_{-\infty}^{\infty} b\left[w(y,t-a)\right] \mathrm{e}^{-(x-y)^2/4Da} \mathrm{d}y. \tag{4.116}$$

If the diffusion coefficient for immature individuals is very small ($D \to 0$), then the Gaussian function in the integrand can be approximated by a Dirac-delta-function,

$$\frac{\partial w}{\partial t} = D\frac{\partial^2 w}{\partial x^2} - \mu w + \int_0^{\infty} \mathrm{d}a f(a) \mathrm{e}^{-\mu a} b\left[w(x,t-a)\right]. \tag{4.117}$$

If there exists only a unique maturation age τ, then $f(a) = \delta(a-\tau)$. Assuming that $b(w) = w\mathrm{e}^{-w}$ we recover Nicholson's equation. Recently, a model consisting of two subpopulations, mature and immature, with an age-dependent disperser–nondisperser transition has been studied analytically and applied to the Neolithic transition in Europe. This model shows good agreement with observational data [292]. This example will be analyzed in detail in Chapter 7.

4.6 Multi-Component Reaction–Diffusion Systems

The reaction–diffusion equations for a system of n species in one-dimensional space read, see Sect. 2.1.2,

$$\frac{\partial \boldsymbol{\rho}}{\partial t} = \mathsf{D}\frac{\partial^2 \boldsymbol{\rho}}{\partial x^2} + \mathbf{F}(\boldsymbol{\rho}), \tag{4.118}$$

where $\boldsymbol{\rho} \in \mathbb{R}^n$, $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$, and D is the $n \times n$ diffusion matrix. We focus on front solutions and illustrate how to determine the front velocity for KPP kinetics. Let us write, for simplicity,

$$F_j(\boldsymbol{\rho}) = c_{jj}(\boldsymbol{\rho})\rho_j + \sum_{m \neq j} \gamma_{jm}\rho_m, \tag{4.119}$$

where $\gamma_{jm} > 0$ for $j \neq m$. The kinetic terms in (4.118) must satisfy the following conditions:

(i) In $\mathbb{R}^n_+ = \left\{\left(\rho_1, \ldots, \rho_n\right) | \rho_j > 0\right\}$, the vector field $\left(F_1(\boldsymbol{\rho}), \ldots, F_n(\boldsymbol{\rho})\right)$ has an unstable stationary state at $\mathbf{0} = (0, \ldots, 0)$ and an asymptotically stable one at $\mathbf{A} = (A_1, \ldots, A_n)$ with $A_j > 0$ for $j = 1, \ldots, n$.
(ii) The coefficients

$$r_j = c_{jj}(\mathbf{0}) = \sup_{0 \le \rho_i \le A_i; \forall i=1,\ldots,n} \left[c_{jj}(\boldsymbol{\rho}) \right] \tag{4.120}$$

must be finite.

4.6.1 Two-Component RD system

In this section we show how to compute the front velocity for a reaction–diffusion system of two components. The calculations can be extended easily to three or more components. Define $\gamma_{12} = \gamma_1$ and $\gamma_{21} = \gamma_2$ for simplicity. Consider the system

$$\frac{\partial \rho_1}{\partial t} = D_1 \frac{\partial^2 \rho_1}{\partial x^2} + f_1(\rho_1, \rho_2)\rho_1 + \gamma_1 \rho_2, \tag{4.121a}$$

$$\frac{\partial \rho_2}{\partial t} = D_2 \frac{\partial^2 \rho_2}{\partial x^2} + f_2(\rho_1, \rho_2)\rho_2 + \gamma_2 \rho_1. \tag{4.121b}$$

We assume that the interaction terms $f_i(\rho_1, \rho_2)$, $i = 1, 2$, are of KPP type. The dynamical behavior of the front is governed by the linear part of the system and we can use the Hamilton–Jacobi formalism, see Sect. 4.2.1. Under the hyperbolic scaling (4.33), the fields $\rho_i^\varepsilon(x,t) = \rho_i(x/\varepsilon, t/\varepsilon)$ satisfy

$$\varepsilon \frac{\partial \rho_1^\varepsilon}{\partial t} = \varepsilon^2 D_1 \frac{\partial^2 \rho_1^\varepsilon}{\partial x^2} + r_1 \rho_1^\varepsilon + \gamma_1 \rho_2^\varepsilon, \tag{4.122a}$$

$$\varepsilon \frac{\partial \rho_2^\varepsilon}{\partial t} = \varepsilon^2 D_2 \frac{\partial^2 \rho_2^\varepsilon}{\partial x^2} + r_2 \rho_2^\varepsilon + \gamma_2 \rho_1^\varepsilon. \tag{4.122b}$$

This system of equations can be rewritten as

$$-A_1 \frac{\partial G^\varepsilon}{\partial t} = D_1 A_1 \left(\frac{\partial G^\varepsilon}{\partial x} \right)^2 - D_1 A_1 \varepsilon \frac{\partial^2 G^\varepsilon}{\partial x^2} + r_1 A_1 + \gamma_1 A_2, \tag{4.123a}$$

$$-A_2 \frac{\partial G^\varepsilon}{\partial t} = D_2 A_2 \left(\frac{\partial G^\varepsilon}{\partial x} \right)^2 - D_2 A_2 \varepsilon \frac{\partial^2 G^\varepsilon}{\partial x^2} + r_2 A_2 + \gamma_2 A_1, \tag{4.123b}$$

after taking into account the nonlinear transformation

$$\rho_i^\varepsilon(x,t) = A_i \exp\left[-\frac{G^\varepsilon(x,t)}{\varepsilon} \right]. \tag{4.124}$$

For simplicity we suppose that the initial conditions for (4.121) have the form

$$\rho_i(x,0) = \begin{cases} A_i, & x < 0, \\ 0, & x \geq 0, \end{cases} \tag{4.125}$$

which will give rise to a front with the minimal propagation velocity. Taking the limit $\varepsilon \to 0$, i.e., the long-time and large-spatial scale limit, we obtain the equation for the action functional $G(x,t)$. Introduction of the definitions (4.38) turns the system (4.123) into an eigenvalue problem $\mathsf{M}\mathbf{A} = H\mathbf{A}$, where

$$\mathsf{M} = \begin{pmatrix} D_1 p^2 + r_1 & \gamma_1 \\ \gamma_2 & D_2 p^2 + r_2 \end{pmatrix}. \tag{4.126}$$

This system of algebraic equations for A_1 and A_2 has a nontrivial solution if $\det(\mathsf{M} - H\mathsf{I}) = 0$:

$$H^2 - H\left(D_1 p^2 + D_2 p^2 + r_1 + r_2\right) + (D_1 p^2 + r_1)(D_2 p^2 + r_2) - \gamma_1\gamma_2 = 0. \tag{4.127}$$

To ensure the positivity of A_1 and A_2, we need to choose the largest eigenvalue $H(p)$, i.e., the largest solution of equation (4.127),

$$H(p) = \frac{D_1 + D_2}{2} p^2 + \frac{r_1 + r_2}{2} + \frac{1}{2}\sqrt{\left[(D_1 - D_2)p^2 + r_1 - r_2\right]^2 + 4\gamma_1\gamma_2}. \tag{4.128}$$

The front velocity can be determined from (4.128) and (4.47). One of the exercises below deals with a particular case where an analytical solution for the front velocity can be obtained.

Exercises

4.1 Find exact solutions for the RD equation with the reaction term $F(\rho) = \rho^{q+1}(1 - \rho^q)$ by looking for solution in the form $\rho(z) = (1 + ae^{bz})^{-s}$ with $z = x - vt$. Determine the unique values for v, b, and s in terms of q. Consider D, a, b, s as positive parameters.

4.2 Consider the RD equation with the piecewise linear emulation for the KPP reaction term

$$F(\rho) = \begin{cases} \alpha\rho, & 0 \leq \rho < a, \\ \beta(1 - \rho), & a < \rho \leq 1, \end{cases} \tag{4.129}$$

with $\beta > 0$. Shift to the traveling wave coordinate and solve the corresponding ordinary differential equation to determine the front profile that satisfies $\rho(-\infty) = 1$ and $\rho(+\infty) = 0$. By matching the derivative of the front profile at $\rho = a$ obtain the front velocity.

4.3 Consider the RD equation with the initial condition

$$\rho(x,0) = \begin{cases} 1, & x < 0, \\ e^{-h(x)}, & x > 0. \end{cases} \tag{4.130}$$

The Hamilton–Jacobi formalism can be extended to incorporate initial condition without compact support by considering

$$G(x,t) = \min_{y \geq 0} \left\{ \varepsilon h(y/\varepsilon) + \int_0^t L(x,s)\mathrm{d}s,\ \ x(t) = x,\ \ x(0) = y \right\}. \tag{4.131}$$

Prove that for $h(x) = \alpha x$ the front velocity is

$$v = \begin{cases} 1/\alpha + \alpha, & \alpha < 1, \\ 2, & \alpha > 1. \end{cases} \tag{4.132}$$

4.4 The equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 (\rho^m)}{\partial x^2} + F(\rho) \tag{4.133}$$

with $F(0) = F(1) = 0$ and $m > 1$ is known as the reaction–diffusion equation in porous media. Transform to the traveling wave coordinate and consider the boundary conditions $\lim_{z \to -\infty} \rho = 1$ and $\lim_{z \to +\infty} \rho = 0$. By defining $q = -\rho^{m-1}\rho_z$ construct a variational principle as in Sect. (4.2.2) to show that

$$v = \max_g 2\sqrt{m} \frac{\int_0^1 \sqrt{\rho^{m-1} F(\rho) g h}\,\mathrm{d}\rho}{\int_0^1 g\,\mathrm{d}\rho}. \tag{4.134}$$

Show that the fronts of the equation (4.133) and those of the equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} + m\rho^{m-1} F(\rho) \tag{4.135}$$

travel with the same velocity.

4.5 The evolution of iodide, I^-, in the iodate–arsenous acid reaction with arsenous acid in stoichiometric excess is well described by the RD equation

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} + (a + b\rho)\rho(c - \rho). \tag{4.136}$$

Here ρ is the concentration of I^-, in M=mol/L, $a = k_a[H^+]^2$, $b = k_b[H^+]^2$, and c is the initial concentration of iodate, $IO_3{}^-$. The experimental values are $k_a = 4.50\times10^3/M^3$ s, $k_b = 4.36\times10^8/M^4$ s, $D = 2.0\times10^{-3}$ mm^2/s, $[H^+] = 7.1\times10^{-3}$ M, and $c = 5.0 \times 10^{-3}$ M. Find the chemically acceptable stationary states of the kinetic term in (4.136) and determine their stability. Show that (4.136) has a propagating front solution connecting the stable to the unstable steady state and determine the propagation velocity v. Compare your value with the experimental value $v_{\text{exp}} = 2.3 \times 10^{-2}$ mm/s.

4.6 Use the variational principle

$$v = \max_g 2\alpha \frac{\int_0^1 \frac{Fg}{\rho(1-\rho)}\mathrm{d}\rho}{\int_0^1 g\mathrm{d}\rho} \tag{4.137}$$

with the trial function $g(\rho) = \exp\left[-\alpha^2 \int \frac{F}{\rho^2(1-\rho)^2}\mathrm{d}\rho\right]$ to calculate the front velocity, connecting 0 and 1, for RD equations with reaction terms given by (a) $b^{-1}\rho(1-\rho)(\rho+b)$, (b) $\rho(1-\rho)(\rho-a)$, and (c) $\rho(1-\rho)$.

4.7 Determine the shift in the front velocity for the RD equation with a Ginzburg–Landau reaction term $F(\rho) = (1-\rho^2)(\rho+a)$ with $0 < a < 1$, when a cutoff is imposed at the metastable state $\rho = -1$.

4.8 Determine the shift in the front velocity for the RD equation with a Nagumo reaction term, when a cutoff is imposed at the state $\rho = 0$. Use the variational principle to show that

$$\delta v = \frac{\sqrt{2}\Gamma(4)a}{\Gamma(1+2a)\Gamma(3-2a)}\varepsilon^{1+2a}. \tag{4.138}$$

4.9 Find the shift in the front velocity for a reaction–diffusion equation where the diffusion coefficient $D(\rho)$ depends on ρ, with $D(0) = 0$, $D'(\rho) > 0$, and the cutoff is imposed at the state $\rho = 0$ of the KPP reaction term.

4.10 Consider the RD equation with the reaction term $F(\rho) = -\rho(\alpha+\rho)$. Since it is always negative, the RD equation cannot have propagating front solutions. Consider that the control parameter α fluctuates around its mean value α_m with a Gaussian noise of zero mean and correlation given by (4.96). Show that if the noise intensity is larger than α_m, the state 0 becomes unstable and can be invaded by a front propagating with the linear velocity.

4.11 Consider the system given in (4.121) with $D_1 = D_2 = D$. Calculate the Hamiltonian and show that it coincides with the Hamiltonian for a single-component RD equation with an effective reaction rate $r = \left(r_1 + r_2 + \sqrt{(r_1 - r_2)^2 + 4\gamma_1\gamma_2}\right)/2$.