Lecture Notes on Mathematical Modelling in the Life Sciences

Benoît Perthame

Parabolic Equations in Biology

Growth, Reaction, Movement and Diffusion

Springer

Lecture Notes on Mathematical Modelling in the Life Sciences

More information about this series at http://www.springer.com/series/10049

Benoît Perthame

Parabolic Equations in Biology

Growth, Reaction, Movement and Diffusion

Springer

Benoît Perthame
Université Pierre et Marie Curie
Paris, France

ISSN 2193-4789 ISSN 2193-4797 (electronic)
Lecture Notes on Mathematical Modelling in the Life Sciences
ISBN 978-3-319-19499-8 ISBN 978-3-319-19500-1 (eBook)
DOI 10.1007/978-3-319-19500-1

Library of Congress Control Number: 2015947290

Springer Cham Heidelberg New York Dordrecht London

Printed on acid-free paper

Springer International Publishing AG Switzerland is part of Springer Science+Business Media (www.springer.com)

Preface

This book is based on lecture notes written for a course I gave at Université Pierre et Marie Curie at the master level (second year); these notes have been extended with more advanced material. They are an attempt to show why Partial Differential Equations (PDEs in short) are used in biology and how one can analytically derive qualitative properties of the solutions, which are relevant for applications. Of course, many types of PDEs are used and these notes are restricted to parabolic equations, while transport equations were already presented in [4].

To give some order to the content, an organizing principle was needed. The leading idea has been to explain in which circumstances the solutions of parabolic equations can exhibit interesting patterns. Indeed, smoothing effects and time decay usually lead to 'flat' solutions. I classify the parabolic equations of interest in Chap. 1, according to two main mathematical structures; Lotka-Volterra equations or reaction-diffusion equations, as they appear in models of chemical reactions. This idea was already present in a course taught by Jost [3] in École Normale Supérieure some years ago and it also leads my progression throughout these notes.

What ingredients are required to explain patterns in reaction-diffusion systems as they are observed in nature? I begin by explaining when patterns cannot occur (when dissipation and relaxation dominates), then I explain gradually the most standard theories of pattern formation. Because of the smoothing properties of the linear heat equation, its solutions cannot exhibit interesting patterns. Nonlinearities are not always sufficient as is shown in Chap. 2; small Lipschitz bounds in bounded domains or entropy properties are major obstacles to pattern formation. The manipulations here are formal; to justify these, careful attention is brought to the notion of weak solutions in Chap. 3.

A first class of problems, leading to interesting behaviors, occurs in the full space because long range propagation phenomena can occur. Already in one space dimension traveling wave solutions are remarkable examples. A very elementary presentation is given in Chap. 4 for the famous models à la Fisher/KPP. The subject has been studied since a long time and more complete texts are [2, 5]. Spikes, spots (in higher dimensions), and pulses are other related patterns, which I present in Chap. 5; when these spots move with instabilities, one can observe various types of patterns that are also presented.

Too large nonlinearities are not an option to generate patterns because blow-up in finite time can occur. This is the matter of Chap. 6 where I present several methods to prove blow-up.

The main method to obtain patterns remains the Turing instability, one of the most counterintuitive results in the theory of PDEs. When the ordinary differential system is stable, diffusion can turn it unstable when diffusion coefficients of the system components are very different. This matter is presented in Chap. 7, with several examples and illustrations.

Fokker-Planck equations are a class of PDEs, which extend the field of reaction-diffusion systems by including drift terms, and which are important for their use in many fields. In particular, because the example of chemotaxis (Keller-Segel system) appears several times in these notes, a general presentation is given in Chap. 8. These are Kolmogorov equations for Stochastic Differential Equations. When jump processes are considered (these also appear in several areas of biology), one arrives at a simpler class of integral equations, which can be handled rigorously; these integral equations also serve to prove existence of solutions of the Fokker-Planck equations by an asymptotic procedure for small jumps. This matter is presented in Chap. 9.

In addition to the derivation of Fokker-Planck equations, small parameters play an important role in pattern formation and lead to an asymptotic analysis of what happens when these small parameters vanish. The mathematical tools to handle this subject are often more advanced (such as viscosity solutions to Hamilton-Jacobi equations [1]) and these notes mention only a few singular perturbation problems. A single example is treated in detail, namely the derivation of the Stefan problem from reaction-diffusion systems. This is performed in Chap. 10.

Besides these singular perturbation problems, and among many others, the use of parabolic equations in tissue growth modeling, in developmental biology and in neurosciences is other important topic that uses material beyond the scope of the present notes.

The material for these notes comes from very different sources, articles, books, courses, conference talks, and discussions. I tried to limit the number of references and I did not try to be exhaustive. I indicate in footnotes some basic articles, hoping that they are sufficient to initiate a search in each particular subject.

Several friends and colleagues gave me some ideas, examples, images, material throughout this course; among them, I thank particularly A. Marrocco for a long collaboration, S.M. Kaber and Y. Deleuze for numerical simulations or pieces of codes based on the software FreeFEM++, F. Hecht (his help was decisive to write an efficient code) and also Simone Séror and Barry Holland who gave several experimental swarming patterns and were very influential in motivating me to develop further mathematical models. I also thank Didier Smets, Dirk Drasdo, Jan Elias, Annie Raoult, and Marie Doumic-Jauffret who provided several contributions to these notes and several students who asked illuminating questions, and gave corrections or comments. Last but not least, Barry Holland read carefully several versions of the manuscript and helped a lot to improve grammar and expression.

Orléans Benoît Perthame
August 22, 2013

References

1. Barles, G.: Solutions de viscosité des équations de Hamilton-Jacobi. Springer, Berlin/Heidelberg (1994)
2. Fife, P.C.: Mathematical Aspects of Reacting and Diffusing Systems. Lecture Notes in Biomathematics. vol. 28, Springer, Berlin (1979)
3. Jost, J.: Mathematical Methods in Biology and Neurobiology. Universitext. Springer (2014)
4. Perthame, B.: Transport Equations Arising in Biology. L. N. Series 'Frontiers in Mathematics'. Birkhauser, Basel (2007)
5. Volpert, A.I., Volpert, V.A., Volpert, V.A.: Traveling Wave Solutions of Parabolic Systems. Translation of Mathematical Monographs, vol. 140, AMS, Providence, RI (1994)

Contents

Chapter 1
Parabolic Equations in Biology

As first examples, we present two general classes of equations that are used in biology: Lotka-Volterra systems and chemical reactions. These are *reaction-diffusion* equations, or in a mathematical classification, semilinear equations. Our goal is to explain what mathematical properties follow from the set-up of the model: nonnegativity properties, monotonicity and entropy inequalities. These are very general examples, for more material and more biologically oriented textbooks, the reader can also consult for instance [2, 4, 13, 15, 16, 19].

1.1 Lotka-Volterra Systems

1.1.1 Movement and Growth

Class I are used in the area of population biology, and ecological interactions, and are characterized by birth and death. For $1 \leq i \leq I$, we denote by $n_i(t,x)$ the population densities of I interacting species at the location $x \in \mathbb{R}^d$ ($d = 2$ for example). We assume that these species move randomly according to Brownian motion with a bias according to a velocity $U_i(t,x) \in \mathbb{R}^d$ and that they have growth rates $R_i(t,x)$ (meaning birth minus death). Then, the system describing the dynamic of these population densities is

$$\frac{\partial}{\partial t} n_i \underbrace{- D_i \Delta n_i}_{\text{random motion}} + \underbrace{\operatorname{div}(U_i n_i)}_{\text{oriented drift}} = \underbrace{n_i\, R_i}_{\text{growth and death}}, \qquad t \geq 0,\ x \in \mathbb{R}^d, \quad i = 1, \dots, I. \tag{1.1}$$

In the simplest cases, the diffusion coefficients $D_i > 0$ are constants depending on the species (they represent active motion of individuals) and the bulk velocity U_i vanishes. Here we insist on the birth and death rates R_i; they depend strongly on the

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_1

interactions between species and we express this fact as a nonlinearity

$$R_i(t,x) = \mathcal{R}_i\big(n_1(t,x), n_2(t,x), \ldots, n_I(t,x)\big). \tag{1.2}$$

A standard family of such nonlinearities results in quadratic interactions and is written

$$\mathcal{R}_i(n_1, n_2, \ldots, n_I) = r_i + \sum_{i=1}^{I} c_{ij} n_j,$$

with r_i the intrinsic growth rate of the species i (it can be positive or negative) and c_{ij} the interaction effect of species j on species i. The coefficients c_{ij} are usually neither symmetric nor nonnegative. One can distinguish

- $c_{ij} < 0$, $c_{ji} > 0$: species i is a prey for j, species j is a predator for i. When several species eat no other food, these are called *trophic* chains/interactions,
- $c_{ij} > 0$, $c_{ji} > 0$: a mutualistic interaction (both species help the other and benefit from it) to be distinguished from symbiosis (association of two species whose survival depends on each other),
- $c_{ij} < 0$, $c_{ji} < 0$: a direct competition (both species compete for example for the same food),
- $c_{ii} < 0$ is usually assumed to represent intra-specific competition.

The quadratic aspect is related to the necessary binary encounters for the interaction to occur. Better models include saturation effects: for instance the effect of too numerous predators is to decrease their individual efficiency. This leads ecologists rather to use (with $\overline{c}_{ii} = -c_{ii} > 0$)

$$\mathcal{R}_i(n_1, n_2, \ldots, n_I) = r_i - \overline{c}_{ii} n_i + \sum_{j=1,\, j\neq i}^{I} c_{ij} \frac{n_j}{1+n_j},$$

the terminology *Holing II* is used in the case where j refers to a prey, i to a predator. Ecological networks are described by such systems: diversity refers to the number of species I itself, connectance refers to the proportion of interacting species, i.e. such that $c_{ij} \neq 0$. Connectance is low for trophic chain and higher for a food web (species use several foods).

The original prey-predator system of Lotka and Volterra has two species, $I = 2$ ($i = 1$ the prey, $i = 2$ the predator). The prey (small fishes) can feed on abundant zooplankton and thus $r_1 > 0$, while predators (sharks) will die out without small fishes to eat ($r_2 < 0$). The sharks eat small fishes in proportion to the number of sharks ($c_{12} < 0$), while the shark population grows proportionally to the small fishes they can consume $c_{21} > 0$). Therefore, we find the rule

$$r_1 > 0, \quad r_2 < 0, \quad c_{11} = c_{22} = 0, \quad c_{12} < 0, \quad c_{21} > 0.$$

1.1.2 Nonnegativity Principle

In all generality, solutions of the Lotka-Volterra system (1.1) satisfy very few qualitative properties; there are neither conservation laws (because they contain birth and death), nor entropy properties, a concept which does not seem to be relevant for ecological systems. As we shall see the quadratic aspect may lead to blow-up (solutions exist only for a finite time, see Chap. 6). Let us only mention here, that the model is consistent with the property that population density be nonnegative.

Lemma 1.1 (Nonnegativity Principle) *Assume that the initial data n_i^0 are nonnegative functions of $L^2(\mathbb{R}^d)$, that $U_i \equiv 0$ and that there is a locally bounded function $\Gamma(t)$ such that $|R_i(t,x)| \leq \Gamma(t)$. Then, the weak solutions in $C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$ to the Lotka-Volterra system (1.1) satisfy $n_i(t,x) \geq 0$.*

The definition and usual properties of weak solutions are given in Chap. 3, but we do not require that theoretical background to show the formal manipulations leading to this result.

Proof (Formal) Here, we use the method of Stampacchia. Set $p_i = -n_i$, then we have

$$\frac{\partial}{\partial t} p_i - D_i \Delta p_i = p_i\, R_i.$$

Multiply by $(p_i)_+ := \max(0, p_i)$ and integrate by parts. We find

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} \big(p_i(t,x)\big)_+^2 dx + D_i \int_{\mathbb{R}^d} \big|\nabla (p_i)_+\big|^2 = \int_{\mathbb{R}^d} \big(p_i(t,x)\big)_+^2 R_i \tag{1.3}$$

and thus

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} \big(p_i(t,x)\big)_+^2 dx \leq \Gamma(t) \int_{\mathbb{R}^d} \big(p_i(t,x)\big)_+^2.$$

Therefore, we have

$$\int_{\mathbb{R}^d} \big(p_i(t,x)\big)_+^2 dx \leq e^{2\int_0^t \Gamma(s) ds} \int_{\mathbb{R}^d} \big(p_i^0(x)\big)_+^2 dx.$$

But, the assumption $n_i^0 \geq 0$ implies that $\int_{\mathbb{R}^d} \big(p_i^0(x)\big)_+^2 dx = 0$, and thus, for all times we have $\int_{\mathbb{R}^d} \big(p_i(t)\big)_+^2 dx = 0$, which means $n_i(t,x) \geq 0$.

(Rigorous) See Sect. 3.7. The difficulty here stems from the "linear" definition of weak solutions of (1.1), which does not allow for nonlinear manipulations such as multiplication by $(p_i)_+$. □

Exercise In the formal context of the Lemma 1.1, show that

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_i(t,x)dx = \int_{\mathbb{R}^d} R_i(t,x)n_i(t,x)dx,$$

$$\int_{\mathbb{R}^d} n_i(t,x)^2dx \le \int_{\mathbb{R}^d} (n_i^0(x))^2dx\; e^{2\int_0^t \Gamma(s)ds}\;.$$

(Left to the reader; see the proof of the Lemma 1.1) in Sect. 3.7. The identity expresses that the total number of individuals only changes according to rates of birth and death, motion does not count.

1.1.3 Operator Monotony for Competition or Cooperative Systems

The positivity property is general but a rather weak property. Comparison principle and monotonicity principle are much stronger properties but require either competition or cooperative systems.

For simplicity we consider only two cooperative species, $I = 2$ in Eqs. (1.1)–(1.2), and we make the cooperative assumption

$$\frac{\partial}{\partial n_2}\mathcal{R}_1(n_1,n_2) \ge 0, \qquad \frac{\partial}{\partial n_1}\mathcal{R}_2(n_1,n_2) \ge 0. \tag{1.4}$$

Lemma 1.2 (Monotonicity Principle) *Consider a cooperative system, that is,* (1.4) *and two solutions n_i, m_i such that for some constants $0 \le n_i \le \Gamma^1$, $0 \le m_i \le \Gamma^1$ and $|\mathcal{R}_i| \le \Gamma^2$, $|\frac{\partial}{\partial n_i}\mathcal{R}_j| \le \Gamma^3$. Then, the Lotka-Volterra system* (1.1)–(1.2) *is ordered for all times*

$$n_i^0 \le m_i^0, \quad i = 1,\ 2 \quad \Longrightarrow \quad n_i(t) \le m_i(t), \qquad \forall t \ge 0,\ i = 1,\ 2.$$

Proof Subtracting the two equations for n_1 and m_1, we find successively, by adding and subtracting convenient terms,

$$\frac{\partial}{\partial t}(n_1-m_1)-D_1\Delta(n_1-m_1) = (n_1-m_1)\mathcal{R}_1(n_1,n_2)+m_1\big(\mathcal{R}_1(n_1,n_2)-\mathcal{R}_1(m_1,m_2)\big),$$

$$\begin{aligned}\frac{\partial}{\partial t}\frac{(n_1-m_1)_+^2}{2} - D_1(n_1-m_1)_+\Delta(n_1-m_1) &= (n_1-m_1)_+^2\mathcal{R}_1(n_1,n_2)\\ &+m_1(n_1-m_1)_+\big(\mathcal{R}_1(n_1,n_2)-\mathcal{R}_1(m_1,n_2)\big)\\ &+m_1(n_1-m_1)_+\big(\mathcal{R}_1(m_1,n_2)-\mathcal{R}_1(m_1,m_2)\big).\end{aligned}$$

The first and second lines are controlled by bounds on $\mathcal{R}$

$$\frac{d}{dt}\int_{\mathbb{R}^d}\frac{(n_1-m_1)_+^2}{2}+D_1\int_{\mathbb{R}^d}|\nabla(n_1-m_1)_+|^2\le(\Gamma^2+\Gamma^1\Gamma^3)\int_{\mathbb{R}^d}(n_1-m_1)_+^2$$
$$+\int_{\mathbb{R}^d}m_1(n_1-m_1)_+\big(\mathcal{R}_1(m_1,n_2)-\mathcal{R}_1(m_1,m_2)\big),$$

We now use $0\le m_1\le\Gamma^1$, $\frac{\partial}{\partial n_2}\mathcal{R}_1(n_1,n_2)\ge 0$ and a Lipschitz constant of $\mathcal{R}_1(n_1,n_2)$, to conclude

$$\frac{d}{dt}\int_{\mathbb{R}^d}\frac{(n_1-m_1)_+^2}{2}\le(\Gamma^2+\Gamma^1\Gamma^3)\int_{\mathbb{R}^d}(n_1-m_1)_+^2+\Gamma^1\Gamma^3\int_{\mathbb{R}^d}(n_1-m_1)_+(n_2-m_2)_+.$$

The same argument on n_2-m_2 leads to the similar inequality

$$\frac{d}{dt}\int_{\mathbb{R}^d}\frac{(n_2-m_2)_+^2}{2}\le(\Gamma^2+\Gamma^1\Gamma^3)\int_{\mathbb{R}^d}(n_2-m_2)_+^2+\Gamma^1\Gamma^3\int_{\mathbb{R}^d}(n_1-m_1)_+(n_2-m_2)_+,$$

and adding these two inequalities, for $u(t)=\int_{\mathbb{R}^d}[(n_1-m_1)_+^2+(n_2-m_2)_+^2]$ and $2ab\le a^2+b^2$, we obtain for some Γ the inequality

$$\frac{du(t)}{dt}\le\Gamma u(t).$$

Since $u(0)=0$ from our initial order assumption, we conclude that $u(t)=0$ for all $t\ge 0$. That is the conclusion of the lemma. □

Exercise Check that for a cooperative system, whatever is its size, the monotony result of Lemma 1.2 holds.

Exercise In the case of 2 by 2 competition systems

$$\frac{\partial}{\partial n_2}\mathcal{R}_1(n_1,n_2)\le 0,\qquad \frac{\partial}{\partial n_1}\mathcal{R}_2(n_1,n_2)\le 0. \tag{1.5}$$

Show that the order $0\le n_1\le m_1$, $0\le m_2\le n_2$ is preserved.

1.1.4 Challenges

Variability There is always a large variability in living populations. For that reason, solutions of models with fixed parameters, for movement or growth, usually fit poorly with experiments or observations. However, the models are useful for explaining qualitatively these observations but not for predicting individual behavior, a major problem when dealing with medical applications for example. A usual point of view is that these parameters are distributed; one can use a statistical representation (see the software Monolix at http://software.monolix.org/) in pharmacology. One can also use so-called structured population models, see [15, 17, 19]. When modeling Darwinian evolution (see adaptive evolution in Sect. 5.1.2), the parameters are part of the model solution and mutations are seen as changes in the model coefficients selected by adaptation to the environment.

Small Numbers In physics and chemistry, 10^{23} is the normal order of magnitude for a number of molecules. Populations that are studied with Lotka-Volterra equations are much smaller and 10^6 is already a large number. This means that exponentially decaying tails are very quickly meaningless because they represent a number of individuals, less than one. The interpretation of such tails should be questioned carefully and several types of corrections can be included; demographic stochasticity is used in Monte-Carlo simulations, which correspond to the survival threshold in PDEs [9].

1.2 Reaction Kinetics and Entropy

When large numbers of molecules are involved in a chemical reaction, the kinetics are well described by *reaction rate equations*. These are nonlinear equations describing the population densities (concentrations) of the reacting molecules and the specific form of these nonlinearities is usually prescribed by the *law of mass action*. This section deals with this aspect of reaction kinetics. The derivation of these equations is postponed to Sect. 9.7 where we introduce the *chemical master equation*, which better describes a small number of reacting molecules, an important topic in cell biology.

1.2.1 Reaction Rate Equations

The General Form of the Equations leads to a particular structure for the right hand side of semi-linear parabolic equations. They are written

$$\frac{\partial}{\partial t} n_i \quad \underbrace{- D_i \Delta n_i}_{\text{molecular diffusion}} \quad + \underbrace{n_i\, L_i \;=\; G_i}_{\text{reaction}}, \qquad t \geq 0,\ x \in \mathbb{R}^d, \quad i = 1, 2, \ldots, I. \tag{1.6}$$

The quantities $n_i \geq 0$ are molecular concentrations, the loss terms $L_i \geq 0$ depend on all the molecules n_j (with which the molecule i can react) and the gain terms $G_i \geq 0$, which also depend on the n_j's, denote the rates of production of n_i from the other reacting molecules. The molecular diffusion rate of these molecules is D_i and can be computed according to the Einstein rule from the molecular size.

For a single reaction, the nonlinearities L_i and G_i take the form

$$n_i L_i = \sum_{\text{reactions } p} k_{pi} \prod_{j=1}^{I} n_j^{a_{pj}}, \qquad G_i = \sum_{\text{reactions } p} k'_{pi} \prod_{j=1}^{I} n_j^{b_{pj}}. \tag{1.7}$$

The powers $a_{pj},\ b_{pj} \in \mathbb{N}$ represent the number of molecules j necessary for the reaction p; this is the *law of mass action*.

Nonnegativity Property We have factored the term n_i in front of L_i to ensure that this term vanishes at $n_i = 0$. The loss term L_i is not singular here because the product contains $\alpha_{pi} \geq 1$ when $k_{pi} > 0$ (the reactant i really reacts). For that reason, as for the Lotka-Volterra systems, the nonnegativity property holds true.

Lemma 1.3 *A weak solution of* (1.6) *with* $G_i \geq 0$ *and nonnegative initial data satisfies* $n_i(t,x) \geq 0$, $\forall i = 1, 2, \ldots, I$.

Proof Adapt the proof of Lemma 1.1.

Even though we do not know that $G_i \geq 0$, this lemma is useful because one may argue as follows. Solutions are first built using the positive part of G_i, then the lemma tells us that the n_i's are positive. From formula (1.7), the positivity of the $n_j's$ implies that G_i is positive and thus that we have built the solution to the correct problem.

Conservation of Atoms The second main property of these models comes from the conservation of atoms, which asserts that some quantities should be constant in time. For each atom $k = 1, \ldots, K$, one defines the number N_{ki} of atoms k in the molecule i. Then all reactions should preserve the number of atoms and, for all $k \in \{1, \ldots, K\}$, the coefficients α, β, k and k' should be such that

$$\sum_{i=1}^{I} N_{ki} \left[n_i \, L_i - G_i \right] = 0, \qquad \forall (n_i) \in \mathbb{R}^I. \tag{1.8}$$

This implies that

$$\frac{\partial}{\partial t} \sum_{i=1}^{I} N_{ki} n_i = \Delta \sum_{i=1}^{I} N_{ki} D_i n_i, \tag{1.9}$$

$$\frac{d}{dt} \int_{\mathbb{R}^d} \sum_{i=1}^{I} N_{ki} n_i(t,x) dx = 0, \qquad 1 \leq k \leq K,$$

and thus, a priori, the weighted L^1 bound holds

$$\int_{\mathbb{R}^d} \sum_{i=1}^{I} N_{ki} n_i(t,x) dx = \int_{\mathbb{R}^d} \sum_{i=1}^{I} N_{ki} n_i^0(x) dx, \qquad 1 \leq k \leq K. \tag{1.10}$$

Except when all the diffusion rates D_i's are equal (then its main part is the heat equation), it is not easy to extract conclusions from Eq. (1.9) except the conservation law (1.10). Very few general tools, such as M. Pierre's duality estimate, are available, see the survey [18].

There is a third property, the entropy dissipation that we shall discuss later.

1.2.2 The Law of Mass Action

Irreversible Reaction To begin with, consider molecular species S_i undergoing the single irreversible reaction

$$a_1 S_1 + \ldots + a_I S_I \xrightarrow{k_+} b_1 S_1 + \ldots + b_I S_I,$$

with $a_i \ , b_i \ \in \ \mathbb{N}$. Then, using the law of mass action, the equation for the concentrations n_i of species i is written

$$\frac{\partial}{\partial t} n_i - D_i \Delta n_i + \underbrace{a_i k_+ \prod_{j=1}^{I} n_j^{a_j}}_{\text{loss of molecules by reaction}} = \underbrace{b_i k_+ \prod_{j=1}^{I} n_j^{b_j}}_{\text{gain of reaction product}}, \qquad i = 1, 2, \ldots, I.$$

From the conservation of atoms, it is impossible that for all i we have $b_i > a_i$ (resp. $a_i < b_i$). Therefore, at least one reactant ($a_i < b_i$) should disappear and one product ($b_i > a_i$) be produced.

Reversible Reaction More interesting is when several reactions occur. Then they are modeled by a sum of such terms over each chemical reaction. For example, still with $a_i \neq b_i \in \mathbb{N}$, the reversible reaction

$$a_1 S_1 + \ldots + a_I S_I \underset{k_-}{\overset{k_+}{\rightleftharpoons}} b_1 S_1 + \ldots + b_I S_I,$$

leads to reaction rate equations

$$\begin{aligned} \tfrac{\partial}{\partial t} n_i - D_i \Delta n_i \quad &+ \overbrace{a_i k_+ \prod_{j=1}^{I} n_j^{a_j}}^{\text{loss of forward reacting molecules}} + \overbrace{b_i k_- \prod_{j=1}^{I} n_j^{b_j}}^{\text{loss of backward reacting molecules}} \\ &= \underbrace{b_i k_+ \prod_{j=1}^{I} n_j^{a_j}}_{\text{gain of forward reaction product}} + \underbrace{a_i k_- \prod_{j=1}^{I} n_j^{b_j}}_{\text{gain of backward reaction product}}. \end{aligned}$$

A more convenient form is

$$\frac{\partial}{\partial t} n_i - D_i \Delta n_i = (b_i - a_i) \left[k_+ \prod_{j=1}^{I} n_j^{a_j} - k_- \prod_{j=1}^{I} n_j^{b_j} \right], \qquad i = 1, 2, \ldots, I. \tag{1.11}$$

With this form, one can check the fundamental *entropy property* for reversible reactions. Define

$$S(t,x) := \sum_{i=1}^{I} n_i \big[\ln(n_i) + \sigma_i - 1 \big], \quad \text{with} \ \sum_{i=1}^{I} \sigma_i (a_i - b_i) = \ln k_+ - \ln k_-. \tag{1.12}$$

There are different possible choices for the constant σ_i, which can be more or less convenient depending on the case. In all cases, one can check the

Lemma 1.4 (Entropy Property for Reversible Reactions) *The entropy dissipation equality holds*

$$\frac{d}{dt} \int S(t,x) dx + \sum_{i=1}^{d} D_i \int \frac{|\nabla n_i|^2}{n_i} dx = -D(t,x) \leq 0,$$

$$D(t,x) := \int \big[\ln(k_+ \prod_{j=1}^{I} n_j^{a_j}) - \ln(k_- \prod_{j=1}^{I} n_j^{b_j}) \big] \big[k_+ \prod_{j=1}^{I} n_j^{a_j} - k_- \prod_{j=1}^{I} n_j^{b_j} \big] \, dx \geq 0.$$

The entropy dissipation property is very important because it dictates the long term behavior of the reaction. Mathematically it is also useful to prove a priori estimates for the quantity $\frac{|\nabla n_i|^2}{n_i}$ but also for integrability properties of powers of n_i, which are necessary to define solutions of the reaction-diffusion equation. This has been used recently in a series of papers by L. Desvillettes and K. Fellner [6] for estimates and relaxation properties, and by T. Goudon and A. Vasseur [12] for regularity properties.

1.2.3 Elementary Examples

Isomerization The reversible isomerization reaction is the simplest chemical reaction. The atoms within the molecule are not changed but only their spatial arrangement. The reaction is represented as

$$S_1 \underset{k_-}{\overset{k_+}{\rightleftharpoons}} S_2$$

and is modeled as

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_+ n_1 = k_- n_2, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + k_- n_2 = k_+ n_1. \end{cases} \tag{1.13}$$

The conserved quantity is simply

$$\frac{d}{dt} \int [n_1(t,x) + n_2(t,x)] dx = 0, \qquad \int [n_1(t,x) + n_2(t,x)] dx = \int [n_1^0(x) + n_2^0(x)] dx.$$

The formula (1.12) for the entropy (with $a_1 = b_2 = 1$, $b_1 = a_2 = 0$) gives

$$S(t,x) = n_1 \big[\ln(k_+ n_1) - 1 \big] + n_2 \big[\ln(k_- n_2) - 1 \big], \tag{1.14}$$

and one can check the entropy dissipation relation

$$\frac{d}{dt} \int_{\mathbb{R}^d} S(t,x) dx = - \int_{\mathbb{R}^d} \big[D_1 \frac{|\nabla n_1|^2}{n_1} + D_2 \frac{|\nabla n_2|^2}{n_2} \big] dx$$
$$- \int_{\mathbb{R}^d} \big[\ln(k_+ \, n_2) - \ln(k_- \, n_1) \big] \big[k_- n_2 - k_+ n_1 \big] \, dx \leq 0.$$

Dioxygen Dissociation The standard degradation reaction of dioxygen to monoxygen is usually associated with hyperbolic models for fluid flows rather than diffusion. This is because it is a very energetic reaction occurring at very high temperature (for atmosphere re-entry vehicles for example) and with reaction rates depending critically on this temperature, see [11]. But for our purpose here, we forget these limitations and consider the dissociation rate $k_+ > 0$ of $n_1 = [O_2]$ in $n_2 = [O]$, and conversely its recombination with rate $k_- > 0$

$$O_2 \underset{k_-}{\overset{k_+}{\rightleftharpoons}} O + O.$$

This leads to

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_+ n_1 = k_- (n_2)^2, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + 2k_- (n_2)^2 = 2k_+ n_1, \end{cases} \tag{1.15}$$

with initial data $n_1^0 \geq 0$, $n_2^0 \geq 0$. According to the *law of mass action*, the term $(n_2)^2$ arises because the encounter of two atoms of monoxygen is required for the reaction.

We derive the conservation law (number of atoms is constant) by a combination of the equations

$$\frac{\partial}{\partial t} [2n_1 + n_2] - \Delta [2D_1 n_1 + D_2 n_2] = 0,$$

which implies that for all $t \geq 0$

$$\int_{\mathbb{R}^d} \big[2n_1(t,x) + n_2(t,x)\big]dx = M := \int_{\mathbb{R}^d} \big[2n_1^0(x) + n_2^0(x)\big]dx. \tag{1.16}$$

For the simple case of the reaction (1.15), the formula (1.12) for the entropy (with $a_1 = 1, b_2 = 2, b_1 = a_2 = 0$) gives

$$S(t,x) = n_1\big[\ln(k_+ n_1) - 1\big] + n_2\big[\ln(k_-^{1/2} n_2) - 1\big]. \tag{1.17}$$

One can readily check that

Lemma 1.5 (Entropy Inequality)

$$\frac{d}{dt}\int_{\mathbb{R}^d} S(t,x)dx = -\int_{\mathbb{R}^d}\big[D_1\frac{|\nabla n_1|^2}{n_1} + D_2\frac{|\nabla n_2|^2}{n_2}\big]dx$$
$$-\int_{\mathbb{R}^d}\big[\ln(k_-\,(n_2)^2) - \ln(k_+\,n_1)\big]\big[k_-(n_2)^2 - k_+ n_1\big]\,dx \leq 0.$$

Exercise Deduce from (1.16) and $n_1 \geq 0$, $n_2 \geq 0$ the a priori bound

$$2k_- \int_0^T \int_{\mathbb{R}^d} (n_2)^2\, dxdt \leq M(1 + 2k_+ T).$$

Hint. In (1.15), integrate the equation for n_1.

Hemoglobin Oxidation Hemoglobin Hb can bind to dioxygen O_2 to form HbO_2 according to the reaction

$$Hb + O_2 \underset{k_-}{\overset{k_+}{\rightleftharpoons}} HbO_2.$$

This reaction is important in brain imaging because the magnetic properties of Hb and HbO_2 are different; the consumption of oxygen by neurones generates deoxyhemoglobin that can be detected by MRI and thus, indirectly, indicates the location of neural activity.

The resulting system of PDEs, for $n_1 = [Hb]$, $n_2 = [O_2]$ and $n_3 = [HbO_2]$, is

$$\begin{cases} \frac{\partial}{\partial t}n_1 - D_1\Delta n_1 + k_+ n_1 n_2 = k_- n_3, \\ \frac{\partial}{\partial t}n_2 - D_2\Delta n_2 + k_+ n_1 n_2 = k_- n_3, \\ \frac{\partial}{\partial t}n_3 - D_3\Delta n_3 + k_- n_3 = k_+ n_1 n_2. \end{cases}$$

From this system, we can derive two conservation laws for the total number of molecules Hb and O_2,

$$\frac{\partial}{\partial t}[n_1 + n_3] - \Delta[D_1 n_1 + D_3 n_3] = 0, \qquad \frac{\partial}{\partial t}[n_2 + n_3] - \Delta[D_2 n_2 + D_3 n_3] = 0.$$

these imply an L^1 control

$$M := \int [n_1(t) + n_2(t) + 2n_3(t)] = \int [n_1^0 + n_2^0 + 2n_3^0].$$

As in the case of dioxygen dissociation, integrating the third equation, one concludes the quadratic estimate

$$k_+ \int_0^\infty \int_{\mathbb{R}^d} n_1 n_2 dx\, dt \le M(1 + k_- T).$$

From (1.12) (with $a_1 = 1, b_2 = 2, b_1 = a_2 = 0$), this also comes with an entropy

$$S(t,x) = n_1[\ln(k_+^{1/2} n_1) - 1] + n_2[\ln(k_+^{1/2} n_2) - 1] + n_3[\ln(k_- n_3) - 1].$$

Mathematical references and studies on this system can be found in B. Andreianov and H. Labani [1].

Exercise Another simple and generic example is the reversible reaction $A + B \underset{k_-}{\overset{k_+}{\rightleftharpoons}} C + D$

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_+ n_1 n_2 = k_- n_3 n_4, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + k_+ n_1 n_2 = k_- n_3 n_4, \\ \frac{\partial}{\partial t} n_3 - D_3 \Delta n_3 + k_- n_3 n_4 = k_+ n_1 n_2, \\ \frac{\partial}{\partial t} n_4 - D_4 \Delta n_4 + k_- n_3 n_4 = k_+ n_1 n_2. \end{cases} \tag{1.18}$$

with the $n_i \ge 0$ and the single atom conservation law

$$\int_{\mathbb{R}^d} \big[n_1(t,x) + n_2(t,x) + n_3(t,x) + n_4(t,x)\big] dx = M$$
$$:= \int_{\mathbb{R}^d} \big[n_1^0(x) + n_2^0(x) + n_3^0(x) + n_4^0(x)\big] dx.$$

Choose k_i so that $S = \sum_{i=1}^{4} n_i \ln(k_i n_i)$ is a convex entropy and write the entropy inequality for the chemical reaction (1.18).

1.2.4 Enzymatic Reactions

More representative of biology are the *enzymatic reactions*, which are usually associated with the names of Michaelis and Menten [14]. A substrate S can be transformed into a product P, without molecular change as in the isomerization reaction, but this reaction occurs only if an enzyme E is present. The process consists first of the formation of a complex SE, that can be itself dissociated into $P+E$. The formation of the complex is a reversible reaction, but the conversion to $P+E$ is an irreversible reaction, leading to the representation

$$S + E \underset{k_-}{\overset{k_+}{\rightleftharpoons}} C = SE \xrightarrow{k_p} P + E.$$

Still using the law of mass action, this leads to the equations (we do not consider the space variable and molecular diffusion, this is not the point here)

$$\begin{cases} \frac{d}{dt}n_S = k_- n_C - k_+ n_S n_E, & \frac{d}{dt}n_E = (k_- + k_p)n_C - k_+ n_S n_E, \\ \frac{d}{dt}n_C = k_+ n_S n_E - (k_- + k_p)n_C, & \frac{d}{dt}n_P = k_p n_C. \end{cases}$$

This reaction comes with the initial data $n_S^0 > 0$, $n_E^0 > 0$ and $n_C^0 = n_P^0 = 0$. One can easily verify that the substrate is entirely converted into the product

$$\lim_{t\to\infty} n_P(t) = n_S^0, \qquad \lim_{t\to\infty} n_S(t) = 0, \quad \lim_{t\to\infty} n_E(t) = n_E^0, \quad \lim_{t\to\infty} n_C(t) = 0.$$

A conclusion that is incorrect if $n_E^0 = 0$. This is a fundamental observation in enzymatic reactions that a very small amount of enzyme is sufficient to convert the substrate into the product.

Two conservation laws hold true in these equations and this helps us to understand the above limit,

$$\begin{cases} n_E(t) + n_C(t) = n_E^0 + n_C^0 = n_E^0, \\ n_S(t) + n_C(t) + n_P(t) = n_S^0 + n_C^0 + n_P^0 = n_S^0. \end{cases} \tag{1.19}$$

Because the properties of the dynamic do not depend on n_P, the system is equivalent to a 2×2 system

$$\begin{cases} \frac{d}{dt}n_S = k_- n_C - k_+ n_S (n_E^0 - n_C), \\ \frac{d}{dt}n_C = k_+ n_S (n_E^0 - n_C) - (k_- + k_p)n_C. \end{cases} \tag{1.20}$$

Briggs and Haldane [3] arrived to the conclusion that this system can be further simplified with the quasi-static approximation on n_C. That means that $n_C(t)$ can be computed algebraically from $n_S(t)$, thus leading to a single ODE for $n_S(t)$

$$\begin{cases} \frac{d}{dt}\overline{n_S} = k_-\overline{n_C} - k_+\overline{n_S}(n_E^0 - \overline{n_C}), \\ 0 = k_+\overline{n_S}(n_E^0 - \overline{n_C}) - (k_- + k_p)\overline{n_C}, \end{cases} \tag{1.21}$$

still with the initial data $\overline{n_S}(t = 0) = n_S^0$ (but no initial condition on n_C). We can of course write this in a more condensed way. Since $\overline{n_C} = \frac{k_+\overline{n_S}n_E^0}{k_-+k_p+k_+\overline{n_S}}$, and after adding the two equations, we find the typical enzymatic reaction kinetic equation

$$\frac{d}{dt}\overline{n_S} = -n_E^0 \frac{k_p k_+\overline{n_S}}{k_- + k_p + k_+\overline{n_S}} \tag{1.22}$$

In other words, the law of mass action does not apply in this approximation and one finds the so-called *Michaelis-Menten law* for the irreversible reactions, a Hill function rather than a polynomial.

Although not obvious at first glance, this result makes rigorous sense and we have the

Proposition 1.6 (Validity of Michaelis-Menten Law) *Assume n_E^0 is sufficiently small. The solutions of* (1.20) *and of* (1.22) *satisfy*

$$\sup_{t\geq 0} |n_S(t) - \overline{n_S}(t)| \leq C(n_S^0)\, n_E^0$$

for some constant $C(n_S^0)$ independent of n_E^0.

Proof We reduce the system to slow-fast dynamic (see [8] for an extended presentation of the subject). To simplify the notations, we set $\varepsilon := n_E^0$ and we define the slow time and new unknowns as

$$\varepsilon := n_E^0, \qquad s = \varepsilon t, \qquad u_S^\varepsilon(s) = n_S(t) \geq 0, \qquad u_C^\varepsilon(s) = \frac{n_C(t)}{n_E^0} \geq 0.$$

Then the two systems are respectively written as

$$\begin{cases} \frac{d}{ds}u_S^\varepsilon = k_-u_C^\varepsilon - k_+u_S^\varepsilon(1-u_C^\varepsilon), \qquad \varepsilon\frac{d}{ds}u_C^\varepsilon = k_+u_S^\varepsilon(1-u_C^\varepsilon) - (k_- + k_p)u_C^\varepsilon, \\ \frac{d}{ds}\overline{u_S} = k_-\overline{u_C} - k_+\overline{u_S}(1-\overline{u_C}), \qquad 0 = k_+\overline{u_S}(1-\overline{u_C}) - (k_- + k_p)\overline{u_C}. \end{cases} \tag{1.23}$$

With these notations the result in Proposition 1.6 is equivalent to

$$\sup_{s\geq 0}|u_S^\varepsilon(s)-\overline{u_S}(t)|\leq C\varepsilon.$$

The details of the proof are left to the reader because it is a general conclusion from the theory of slow-fast dynamic. We shall make use of the two consequences of (1.23)

$$\frac{d}{ds}[u_S^\varepsilon+\varepsilon u_C^\varepsilon]=-k_p u_C^\varepsilon, \qquad\qquad \frac{d}{ds}\overline{u_S}=-k_p\overline{u_C}.$$

We have from (1.19) and $u_C^\varepsilon(t=0)=0$,

(i) $0\leq u_C^\varepsilon\leq 1, \qquad 0\leq \overline{u_C}\leq 1$,
(ii) $0\leq u_S^\varepsilon\leq n_S^0, \qquad 0\leq \overline{u_S}\leq n_S^0$,
(iii) $0\leq u_C^\varepsilon\leq u^M<1, \qquad 0\leq\overline{u_C}\leq u^M<1 \qquad$ with $u^M:=\frac{k_+n_S^0}{k_+n_S^0+k_-+k_p}$ independent of ε,
(iv) $|\frac{d}{ds}u_C^\varepsilon(s)|\leq K$ for some $K(n_S^0)$,
(v) From step (iv), introduce the bounded quantity $r^\varepsilon(s):=-\frac{d}{ds}u_C^\varepsilon(s)+k_+u_C^\varepsilon(s)^2$, and

$$R^\varepsilon(s)=u_S^\varepsilon(s)+\varepsilon u_C^\varepsilon(s)-\overline{u_S}(s).$$

Compute that

$$u_C^\varepsilon(s)=\frac{\varepsilon r^\varepsilon(s)-k_+u_C^\varepsilon R^\varepsilon+k_+u_S^\varepsilon}{k_+\overline{u_S}+k_-+k_p},$$

$$u_C^\varepsilon-\overline{u_C}=\frac{\varepsilon r^\varepsilon+k_+(1-u_C^\varepsilon)R^\varepsilon-\varepsilon k_+u_C^\varepsilon}{k_+\overline{u_S}+k_-+k_p}.$$

Conclude that

$$\frac{d}{ds}R^\varepsilon(s)+k_p\,\frac{k_+(1-u_C^\varepsilon)}{k_+\overline{u_S}+k_-+k_p}\,R^\varepsilon(s)=\varepsilon k_p\frac{-r^\varepsilon+k_+u_C^\varepsilon}{k_+\overline{u_S}+k_-+k_p}.$$

(vi) Using steps (iii) and (v), conclude that $|R^\varepsilon(s)|\leq C\varepsilon$ for a constant C.

Hints.

(ii) $u_S^\varepsilon+u_C^\varepsilon$ decreases.
(iii) Write $\frac{d}{ds}u_C^\varepsilon\leq k_+n_S^0(1-u_C^\varepsilon)-(k_-+k_p)u_C^\varepsilon$.
(iv) Write the equation for $z(s)=\frac{d}{ds}u_C^\varepsilon(s)$ as $\varepsilon\frac{d}{ds}z+\lambda(s)z(s)=\mu(s)$ with $\lambda>k_-+k_p$ and μ bounded.
(vi) Write $\frac{1}{2}\frac{d}{ds}R^\varepsilon(s)^2+AR^\varepsilon(s)^2\leq\varepsilon B|R^\varepsilon(s)|$, with $A>0$, $B>0$ two constants.

1.2.5 Belousov-Zhabotinskii Reaction

For all complex chemical reactions, the detailed description of all elementary reactions is not realistic. Then, as for the enzymatic reaction, one simplifies the system by assuming that some reactions are much faster than others, or that some components are in higher concentrations than others. These manipulations may violate mass conservation and entropy inequality may be lost; this is a condition to obtain pattern formation as in the example of the CIMA reaction in Sect. 7.5.2.

The famous Belousov-Zhabotinskii reaction is known as the first historical example to produce periodic patterns. This was discovered in 1951 by Belousov, it remained unpublished because no respectable chemist at that time could accept this idea. Belousov received the Lenin Prize in 1980, a decade after his death and the discovery in the USA of other periodic reactions, simpler to reproduce.

We borrow a simple example from A. Turner [20], this avoids entering the details of a real chemical reaction (refer to [15] for a complete treatment). The simple example consists of three reactants denoted as A, B, C, and three irreversible reactions (because of this feature, entropy dissipation and relaxation do not hold).

$$A + B \xrightarrow{k_A} 2A, \qquad B + C \xrightarrow{k_B} 2B, \qquad C + A \xrightarrow{k_C} 2C.$$

Therefore, the systems is written as

$$\begin{cases} \frac{d}{dt} n_A = n_A(k_A n_B - k_C n_C), \\ \frac{d}{dt} n_B = n_B(k_B n_C - k_A n_A), \\ \frac{d}{dt} n_C = n_C(k_C n_A - k_B n_B). \end{cases} \tag{1.24}$$

Numerical simulations are presented in Fig. 1.1.

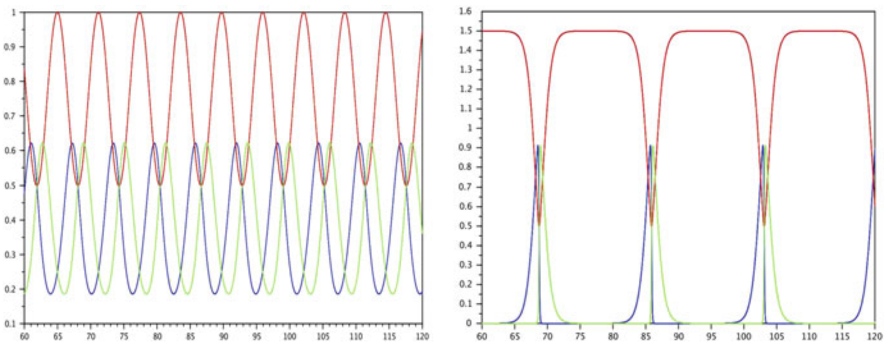

Fig. 1.1 Periodic regime of the system of ODEs (1.24) that mimics the Belousov-Zhabotinskii reaction. The parameters are $k_A = k_B = 1$ and $k_C = 2$ (*Left*), $k_C = 20$ (*Right*). The solution n_C is the *top (red) curve*. In abscissae is time

1.2.6 Small Numbers of Molecules

It may happen that in biological systems, e.g. intracellular bio-molecular interactions, the number of molecules is not large so that the reaction rate equations are not applicable. The alternative is to use the so-called *chemical master equations* that describe the dynamic of individual molecules.

These models are close to the jump processes described in Chap. 9 and with a brief presentation in Sect. 9.7. They allow for a number of asymptotic limits (from discrete to continuous, from continuous jumps to drift-diffusion). For these reasons, there is a large literature on this subject, on both the theoretical and numerical aspects [5, 7, 10].

1.3 Boundary Conditions

When working in a domain (a connected open set with sufficiently smooth boundary) Ω, we encounter two elementary types of boundary conditions. The reaction-diffusion systems (1.1) or (1.6) are completed either by

- **Dirichlet boundary conditions** $n_i = 0$ on $\partial\Omega$. This means that individuals or molecules cross the boundary and do not come again in Ω. This interpretation stems from the Brownian motion underlying the diffusion equation. But we can see that indeed, if we consider the conservative chemical reactions (1.6) with (1.8), then

$$\frac{d}{dt}\int_{\Omega}\sum_{i=1}^{I} n_i(t,x)dx = \sum_{i=1}^{I} D_i \int_{\partial\Omega} \frac{\partial}{\partial\nu} n_i,$$

  with ν the outward normal to the boundary. But with $n_i(t,x) \geq 0$ in Ω and $n_i(t,x) = 0$ in $\partial\Omega$, we have $\frac{\partial}{\partial\nu} n_i \leq 0$, therefore the total mass diminishes

$$\int_{\Omega}\sum_{i=1}^{I} n_i(t,x)dx \leq \int_{\Omega}\sum_{i=1}^{I} n_i^0(x)dx, \qquad \forall t \geq 0.$$

- **Neumann boundary conditions** $\frac{\partial}{\partial\nu} n_i = 0$ on $\partial\Omega$, still with ν the outward normal to the boundary. This means that individuals or molecules are deflected when they hit the boundary. In the computation above for (1.6) with (1.8), the normal derivative vanishes and we find directly mass conservation

$$\int_{\Omega}\sum_{i=1}^{I} n_i(t,x)dx = \int_{\Omega}\sum_{i=1}^{I} n_i^0(x)dx.$$

There is a large difference between the case of the full space $\mathbb{R}^d$ and the case of a bounded domain. This can be seen by the results of spectral analysis in Sect. 2.5, which do not hold in the same form in $\mathbb{R}^d$ and is replaced by Fourier transform.

1.4 Brownian Motion and the Heat Equation

The relationship between Brownian motion and the heat equation explains, in a simple framework, why a random walk of individuals leads to the terms $-D\Delta n$ for the population density $n(t,x)$. It is rather abstract to construct rigorously Brownian motion. However, it is easy to give an intuitive approximation, which is sufficient to build the probability law of Brownian trajectories.

To do so, we follow the Euler numerical method for an ODE with a time step Δt that uses discrete times $t^k = k\Delta t$.

In a probability space with a measure denoted $dP(\omega)$, the initial position $X^0 \in \mathbb{R}^d$ being given with a probability law $n^0(x)$, we define iteratively a discrete trajectory $X^k(\omega) \in \mathbb{R}^d$ as follows. We set

$$X^{k+1}(\omega) = X^k(\omega) + \sqrt{\Delta t}\, Y^k(\omega) \tag{1.25}$$

where $Y^k(\omega)$ denotes a d-dimensional random variable *independent* of X^k (one speaks of independent increments) and with a normal law $N(y)$. We recall that 'independent' means

$$\mathbb{E}f(X^k, Y^k) := \int f\big(X^k(\omega), Y^k(\omega)\big)dP(\omega) = \int_{\mathbb{R}^d\times\mathbb{R}^d} f(x,y)dn^k(x)\, N(y)dy \tag{1.26}$$

with

- $N(y) = \frac{1}{(2\pi)^{d/2}} e^{-|y|^2/2}$, the normal law,
- $dn^k(x)$ the law of the process X^k, defined as $P\big(\Phi(X^k(\cdot))\big) = \int \Phi(x)dn^k(x)$.

Two simulations are presented. Figure 1.2 depicts, in the one dimensional case (t^k, X^k), two iterates X^k (for two different ω). Figure 1.3 shows two iterates X^k in two dimensions.

Our purpose is to compute the law $dn^k(x)$ at the limit $\Delta t \to 0$. To do so, we first use a C^3 function u, with u, Du, D^2u and D^3u bounded. We use the Taylor expansion of u to compute

$$u(X^{k+1}) = u(X^k) + \sqrt{\Delta t} Du(X^k).Y^k + \frac{\Delta t}{2} D^2u(X^k).(Y^k, Y^k) + O\big(\Delta t|Y^k|\big)^{3/2},$$

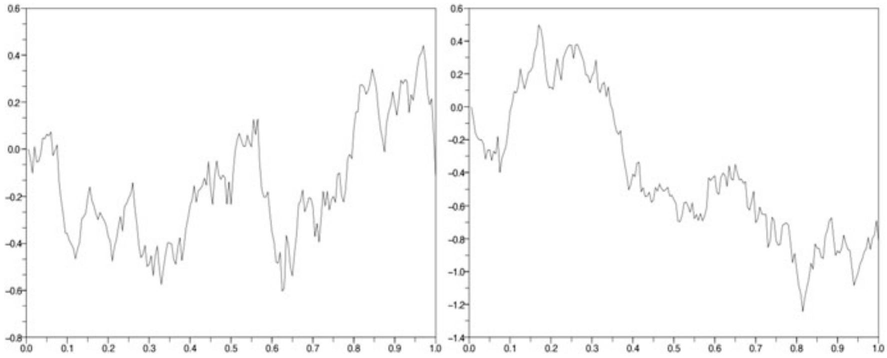

Fig. 1.2 Two sample paths of one dimensional Brownian motion according to the approximation (1.25). Abscissae t^k, ordinates X^k

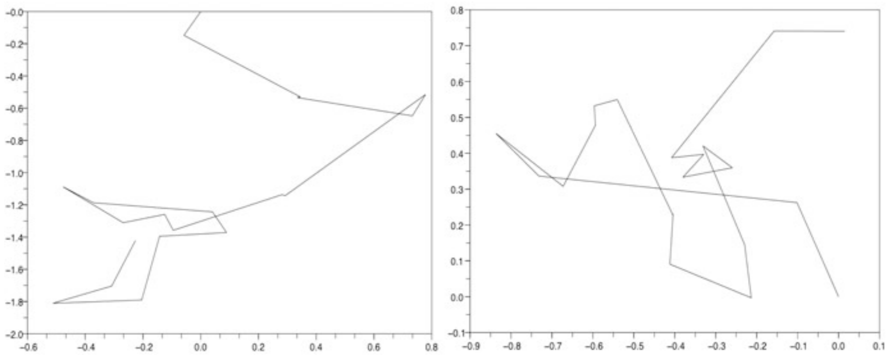

Fig. 1.3 Two sample paths of two dimensional Brownian motion simulated according to (1.25)

and then

$$\mathbb{E}u(X^{k+1}) = \mathbb{E}u(X^k) + \frac{\Delta t}{2}\mathbb{E}D^2u(X^k).(Y^k, Y^k) + O\big(\Delta t\big)^{3/2}. \tag{1.27}$$

Indeed, because $N(\cdot)$ is radially symmetric, the formula (1.26) used with $f(x, y) = Du(X^k).Y^k$ yields

$$\mathbb{E}Du(X^k).Y^k = \mathbb{E}Du(X^k).\int_{\mathbb{R}^d} yN(y)dy = 0.$$

Because $\int_{\mathbb{R}^d} y_i y_j N(y)dy = \delta_{ij}$, a further use of the formulas (1.27), (1.26) and the definition of the probability law mentioned earlier, give

$$\int_{\mathbb{R}^d} u(x)dn^{k+1}(x) = \int_{\mathbb{R}^d} u(x)dn^k(x) + \frac{\Delta t}{2}\int_{\mathbb{R}^d} \Delta u(x)dn^k(x) + O\big(\Delta t\big)^{3/2}.$$

After dividing by Δt and integration by parts of the term Δu, we may rewrite this as

$$\int_{\mathbb{R}^d} u \, \Big[\frac{dn^{k+1} - dn^k}{\Delta t} - \frac{1}{2}\Delta dn^k\Big] = O\big(\Delta t\big)^{1/2}.$$

This holds true for any smooth function u and this means that, in the weak sense,

$$\frac{dn^{k+1} - dn^k}{\Delta t} - \frac{1}{2}\Delta dn^k = O\big(\Delta t\big)^{1/2}.$$

At the limit in the sense of distributions, as $\Delta t \to 0$, we obtain a probability law with a density $n(t,x)$ that satisfies

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \frac{1}{2}\Delta n(t,x) = 0, \\ n(0,x) = n^0(x). \end{cases}$$

In particular, even though n^0 is a probability measure, it follows from the regularizing effects of the heat equation that $n(t,x)$ is a (smooth) function and not only a measure as soon as $t > 0$.

The equation for $n(t,x)$ (the heat equation here) is generically called the Kolmogorov equation for the limiting process (Brownian motion).

Exercise Prove that the density of the probability law n^k satisfies the integral equation

$$n^{k+1}(x) - n^k(x) = \int \big[n^k(x + \sqrt{\Delta t}\, y) - n^k(x)\big] N(y) dy. \tag{1.28}$$

Derive the heat equation for the limit $n(t,x)$, as $\Delta t \to 0$, if it exists. Show that this derivation uses only two y-moments of N and not the full normal law.

See also the scattering equation in Chap. 9.

References

1. Andreianov, B., Labani, H.: Preconditioning operators and L^∞ attractor for a class of reaction-diffusion systems. Commun. Pure Appl. Anal. **11**(6), 2179–2199 (2012)
2. Baker, R.E., Gaffney, E.A., Maini, P.K.: Partial differential equations for self-organization in cellular and developmental biology. Nonlinearity **21**, R251–R290 (2008)
3. Briggs, G.E., Haldane, J.B.S.: A note on the kinematics of enzyme action. Biochem. J. **19**, 338–339 (1925)
4. Cantrell, R.S., Cosner, C.: Spatial Ecology via Reaction–Diffusion Equations. Wiley, Sussex (2003)
5. De Masi, A., Presutti, E.: Mathematical Methods for Hydrodynamic Limits. Springer, Berlin (1991)

6. Desvillettes, L., Fellner, K.: Entropy methods for reaction-diffusion equations: slowly growing a-priori bounds. Rev. Mat. Iberoam. **24**(2), 407–431 (2008)
7. Doob, J.-L.: Markoff chains - Denumerable case. Trans. Am. Math. Soc. **58**(3), 455–473 (1945)
8. Françoise, J.-P.: Oscillations en biologie. Collection Mathématiques et Applications. SMAI, Springer, Paris (2005)
9. Gauduchon, M., Perthame, B.: Survival thresholds and mortality rates in adaptive dynamic: conciliating deterministic and stochastic simulations. Math. Med. Biol. **27**(3), 195–210 (2010)
10. Gillespie, D.T.: Exact stochastic simulation of coupled chemical reactions. J. Phys. Chem. **81**(25), 2340–2361 (1977)
11. Godlewski, E., Raviart, P.-A.: Numerical Approximation of Hyperbolic Systems of Conservation Laws. Applied Mathematical Sciences, vol. 118. Springer, New York (1996)
12. Goudon, T., Vasseur, A.: Regularity analysis for systems of reaction-diffusion equations. Ann. l'ENS **43**(1), 117–141 (2010)
13. Keener, J., Sneyd, J.: Mathematical Physiology. Springer, Heidelberg (2008)
14. Michaelis, L., Menten, M.I.: Die kinetic der invertinwirkung. Biochem. Z. **49**, 333–369 (1913)
15. Murray, J.D.: Mathematical Biology, vols. 1 and 2, 2nd edn. Springer, New York (2002)
16. Okubo, A., Levin, S.A. (eds.): Diffusion and Ecological Problems, Modern Perspectives, 2nd edn. Springer, New York (2001)
17. Perthame, B.: Transport Equations Arising in Biology. L. N. Series Frontiers in Mathematics. Birkhauser, Basel (2007)
18. Pierre, M.: Global existence in reaction-diffusion systems with control of mass: a survey. Milan J. Math. **78**(2), 417–455 (2010)
19. Thieme, H.R.: Mathematics in Population Biology. Woodstock Princeton University Press, Princeton (2003)
20. Turner, A.: A Simple Model of the Belousov-Zhabotinsky Reaction from First Principles. http://www.aac.bartlett.ucl.ac.uk/processing/samples/bzr.pdf (2009)

Chapter 2
Relaxation, Perturbation and Entropy Methods

Solutions of nonlinear parabolic equations and systems presented in Chap. 1 can exhibit various and sometimes complex behavior, a phenomena usually called *pattern formation*. In which circumstances can such complex behavior happen? A first answer is given in this chapter by indicating some conditions for relaxation to trivial steady states; then nothing interesting can happen! We present relaxation results by perturbation methods (small nonlinearity) and entropy methods. Indeed, before we can understand how patterns occur in parabolic systems, a necessary step is to understand why patterns should not appear in principle! Solutions of parabolic equations undergo regularization effects that lead them to constant or simple states. Several asymptotic results can be stated in this direction and we present some of them in this chapter. Sections 2.1 and 2.2 have been very much influenced by the book [4].

2.1 Asymptotic Stability by Perturbation Methods (Dirichlet)

The simplest possible long term behavior for a semilinear parabolic equation is simply the relaxation towards a stable steady state (that we choose to be 0 here). This is possible when the following two features are combined

- the nonlinear part is a *small* perturbation of a main (linear differential) operator,
- this main linear operator has a positive dominant eigenvalue.

Of course this simple relaxation behavior is rather boring and appears as the opposite of pattern formation when Turing instability occurs, and this will be described later, see Chap. 7.

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_2

To illustrate this, we consider, in a bounded domain Ω, the semi-linear heat equation with a Dirichlet boundary condition

$$\begin{cases} \frac{\partial}{\partial t} u_i(t,x) - D_i \Delta u_i(t,x) = F_i(t,x;u_1,\dots,u_I), \qquad 1 \le i \le I, \quad x \in \Omega, \\ u_i(t,x) = 0, \qquad x \in \partial\Omega, \\ u_i(t=0,x) = u_i^0(x) \in L^2(\Omega). \end{cases} \tag{2.1}$$

We assume that $F(t,x;0) = 0$, so that $u \equiv 0$ is a steady state solution. Is it a stable and attractive state?

We shall use here a technical result. The Laplace operator (with Dirichlet boundary condition) has a first eigenvalue $\lambda_1 > 0$, associated with a positive eigenfunction, $w_1(x)$, which is unique except multiplication by a constant,

$$-\Delta w_1 = \lambda_1 \, w_1, \qquad w_1 \in H_0^1(\Omega). \tag{2.2}$$

This eigenvalue is characterized as being the best constant in the Poincaré inequality (see Sect. 2.5 or the book [2])

$$\lambda_1 \int_\Omega |v(x)|^2 \le \int_\Omega |\nabla v|^2, \qquad \forall v \in H_0^1(\Omega),$$

with equality only for $v = \mu w_1$, $\mu \in \mathbb{R}$.

Theorem 2.1 (Asymptotic Stability) *Assume* $\min_i D_i = d > 0$ *and that there is a (small) constant* $L > 0$ *such that* $\forall u \in \mathbb{R}^I, \ t \ge 0, \ x \in \Omega$,

$$|F(t,x;u)| \le L|u|, \quad \textit{or more generally,} \quad F(t,x;u)\cdot u \le L\,|u|^2\,, \tag{2.3}$$

$$\delta = d\lambda_1 - L > 0, \tag{2.4}$$

then, $u_i(t,x)$ *vanishes exponentially as* $t \to \infty$, *namely,*

$$\int_\Omega |u(t,x)|^2 \le e^{-2\delta t} \int_\Omega |u^0(x)|^2. \tag{2.5}$$

Proof We multiply the parabolic equation (2.1) by u_i and integrate by parts

$$\frac{1}{2}\frac{d}{dt}\int_\Omega u_i(t)^2 + D_i \int_\Omega \left|\nabla u_i(t)\right|^2 = \int_\Omega u_i(t) F_i\big(t,x;u(t)\big),$$

and using the characterization (2.2) of λ_1, we conclude

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \sum_{i=1}^I u_i(t)^2 + d\lambda_1 \int_\Omega \sum_{i=1}^I u_i(t)^2 \le L \int_\Omega \sum_{i=1}^I u_i(t)^2.$$

The result follows from the Gronwall lemma. □

Exercise Consider a smooth bounded domain $\Omega \subset \mathbb{R}^d$, a real number $\lambda > 0$ and two smooth and Lipschitz continuous functions $R(u, v), Q(u, v)$, such that $R(0, 0) = Q(0, 0) = 0$. Let $\big(u(x, t), v(x, t)\big)$ be solutions of the system

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = R(u(x,t), v(x,t)), & t \geq 0,\ x \in \Omega, \\ u(x,t) = 0 \quad \text{sur } \partial\Omega, & \\ \frac{\partial}{\partial t}v + \lambda v = Q(u(x,t), v(x,t)). & \end{cases}$$

1. Recall the Poincaré inequality for u.
2. Assume $|R(u, v)| \leq L(|u|+|v|)$ and $|Q(u, v)| \leq L(|u|+|v|)$, give a size condition for L such that for all initial data, the solution (u, v) converges exponentially to $(0, 0)$ for $t \to \infty$.

Solution A simple answer is $\min(\lambda_1, \mu) - 2L =: \delta > 0$. A more elaborate condition is based on the positive real number such that $\lambda_1 - \mu = a - a^{-1}$ and is $\lambda_1 - L - a^{-1} = \mu - L - a =: \delta > 0$.

2.2 Asymptotic Stability by Perturbation Methods (Neumann)

The next simplest possible long term behavior for a parabolic equation is relaxation towards an homogeneous (i.e., independent of x) solution, which is not constant in time. This is possible when two features are combined

- the nonlinear part is a *small* perturbation of a main (differential) operator,
- this main operator has a non-empty kernel (0 is the first eigenvalue).

Consider again, in a bounded domain Ω with outward unit normal ν, the semilinear parabolic equation with a Neumann boundary condition

$$\begin{cases} \frac{\partial}{\partial t}u_i(t,x) - D_i\Delta u_i(t,x) = F_i(t; u_1, \ldots, u_I), & 1 \leq i \leq I, \quad x \in \Omega, \\ \frac{\partial}{\partial \nu(x)}u_i(t,x) = 0, \qquad x \in \partial\Omega, & \\ u_i(t=0,x) = u_i^0(x) \in L^2(\Omega). & \end{cases} \tag{2.6}$$

The Laplace operator (with a Neumann boundary condition) has $\lambda_1 = 0$ as a first eigenvalue, associated with the constants $w_1(x) = 1/\sqrt{|\Omega|}$ as eigenfunction. We shall use its second eigenvalue λ_2, characterized by the Poincaré-Wirtinger inequality (see [2] and Sect. 2.5)

$$\lambda_2 \int_\Omega |v(x) - \langle v\rangle|^2 \leq \int_\Omega |\nabla v|^2, \qquad \forall v \in H^1(\Omega), \tag{2.7}$$

with the average of $v(x)$ defined as

$$\langle v \rangle = \frac{1}{|\Omega|} \int_\Omega v.$$

Note that this is also the L^2 projection on the eigenspace spanned by w_1.

Theorem 2.2 (Relaxation to a Homogeneous Solution) *Assume* $\min_i D_i = d > 0$ *and*

$$\big(F(u) - F(v)\big) \cdot (u - v) \le L\,|u - v|^2, \qquad \forall u,\ v \in \mathbb{R}^I, \tag{2.8}$$

$$\delta = d\lambda_2 - L > 0, \tag{2.9}$$

then, $u_i(t,x)$ *tends to become homogeneous with an exponential rate, namely,*

$$\int_\Omega |u(t,x) - \langle u(t) \rangle|^2 \le e^{-2\delta t} \int_\Omega |u^0(x) - \langle u^0 \rangle|^2. \tag{2.10}$$

Proof Integrating in x Eq. (2.6), we find

$$\frac{d}{dt} \langle u_i \rangle = \langle F_i(t;u) \rangle,$$

therefore,

$$\frac{d}{dt}[u_i - \langle u_i \rangle] - D_i \Delta [u_i - \langle u_i \rangle] = F_i(t;u) - \langle F_i(t;u) \rangle.$$

Thus, using assumption (2.8), we find

$$\begin{aligned}
\tfrac{1}{2}\tfrac{d}{dt} \int_\Omega |u - \langle u \rangle|^2 + d \int_\Omega |\nabla\big(u - \langle u \rangle\big)|^2 &= \int_\Omega \big(F(t;u) - \langle F(t;u) \rangle\big) \cdot (u - \langle u \rangle) \\
&= \int_\Omega F(t;u) \cdot (u - \langle u \rangle) \\
&= \int_\Omega \big(F(t;u) - F(t;\langle u \rangle)\big) \cdot (u - \langle u \rangle) \\
&\le L \int_\Omega |u - \langle u \rangle|^2.
\end{aligned}$$

Therefore, with notation (2.9)

$$\frac{d}{dt} \int_\Omega |u - \langle u \rangle|^2 \le -2\delta \int_\Omega |u - \langle u \rangle|^2.$$

The result (2.10) follows directly. □

Exercise Explain why we cannot allow a dependency on x in the nonlinearity $F_i(t;u)$.

Exercise Let $v \in H^2(\Omega)$ satisfy $\frac{\partial v}{\partial \nu} = 0$ on $\partial\Omega$ (Neumann condition).

1. Prove, using the Poincaré-Wirtinger inequality (2.7), that

$$\lambda_2 \int_\Omega |\nabla v|^2 \leq \int_\Omega |\Delta v|^2. \tag{2.11}$$

2. In the context of Theorem 2.2, assume that $\sum_{i,j=1}^{I} D_j F_i(t;u)\xi_i\xi_j \leq L|\xi|^2$, $\forall \xi \in \mathbb{R}^I$.

   Using the above inequality, prove that

$$\int_\Omega \sum_i |\nabla u_i(t,x)|^2 \leq e^{-2\delta t} \int_\Omega \sum_i |\nabla u_i^0(x)|^2. \tag{2.12}$$

3. Deduce a variant of Theorem 2.2.

   Hints. 1. Integrate by parts the expression $\int_\Omega |\nabla v|^2$. 2. Use the equation for $\frac{d}{dt}\frac{\partial u_i}{\partial x_l}$.

2.3 Entropy and Relaxation

We have seen in Lemma 1.5 that reaction kinetic equations as in (1.15) are endowed with an entropy (1.17). This originates from the microscopic N-particle stochastic systems from which reaction kinetics are derived (see Sect. 9.7).

This entropy inequality is also very useful because it can be used to show relaxation to the steady state, independently of the size of the constants k_1, k_2. To do that we consider a Neumann boundary condition in a bounded domain Ω

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_1 n_1 = k_2 (n_2)^2, & t \geq, \ x \in \Omega, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + 2k_2 (n_2)^2 = 2k_1 n_1, & \\ \frac{\partial}{\partial \nu} n_1 = \frac{\partial}{\partial \nu} n_2 = 0 \qquad \text{on } \ \partial\Omega. & \end{cases} \tag{2.13}$$

Theorem 2.3 *The solutions of* (2.13)*, with* $n_i^0 \geq 0$*,* $n_i^0 \in L^1(\Omega)$*,* $n_i^0 \ \ln(n_i^0) \in L^1(\Omega)$*, satisfy that*

$$n_i(t,x) \to N_i, \qquad as \ \ t \to \infty$$

with N_i *the constants defined uniquely by*

$$2N_1 + N_2 = \int_\Omega [2n_1^0(x) + n_2^0(x)]dx, \qquad k_2(N_2)^2 = k_1 N_1.$$

Proof We give a formal proof since we do not justify the nonlinear manipulations. Then $S(t,x) = n_1\big[\ln(k_1 n_1)-1\big]+n_2\big[\ln(k_2^{1/2} n_2)-1\big]$ satisfies, following Lemma 1.5,

$$\frac{d}{dt}\int_\Omega S(t,x)dx = \int_\Omega \big[D_1 \tfrac{|\nabla n_1|^2}{n_1} + D_2 \tfrac{|\nabla n_2|^2}{n_2}\big]dx$$
$$+ \int_\Omega \big[\ln(k_2\, n_2^2) - \ln(k_1\, n_1)\big]\big[k_2(n_2)^2 - k_1 n_1\big]\, dx.$$

And, because S is bounded from below, it also gives a bound on the entropy dissipation

$$\int_0^\infty \int_\Omega \big[D_1 \tfrac{|\nabla n_1|^2}{n_1} + D_2 \tfrac{|\nabla n_2|^2}{n_2}\big]dxdt$$
$$+ \int_0^\infty \int_\Omega \big[\ln(k_2\, n_2^2) - \ln(k_1\, n_1)\big]\big[k_2(n_2)^2 - k_1 n_1\big]\, dxdt \le C(n_1^0, n_2^0). \tag{2.14}$$

This is again a better integrability estimate in x than the $L^1_{\log}$ estimate (derived from mass conservation) because of the quadratic term $(n_2)^2$.

From a qualitative point of view, this says that the chemical reaction should lead the system to a spatially homogeneous equilibrium state. Indeed, formally at least, the integral (2.14) can be bounded only if

$$\nabla n_1 = \nabla n_2 \approx 0 \qquad \text{as } \ t \to \infty,$$

$$k_2(n_2)^2 \approx k_1 n_1, \quad \nabla n_1 = \nabla n_2 \approx 0 \qquad \text{as } \ t \to \infty.$$

The first conclusion says that the dynamic becomes homogeneous in x (but may depend on t). The second conclusion, combined with the mass conservation relation (1.16) shows that there is a unique possible asymptotic homogeneous state because the constant state satisfies $k_2(N_2)^2 = k_1 N_1 = k_1(\frac{M}{|\Omega|} - N_2)$, which has a unique positive root. □

Exercise Consider (1.15) with a Neumann boundary condition and set

$$S(t,x) = \frac{1}{k_1}\Sigma_1\big(k_1 n_1(t,x)\big) + \frac{1}{2k_2^{1/2}}\Sigma_2\big(k_2^{1/2} n_2(t,x)\big).$$

1. We assume that Σ_1, Σ_2 satisfy $\Sigma_1'(u) = \Sigma_2'(u^{1/2})$. Show that Σ_1 is convex if, and only if, Σ_2 is convex.
2. Under the conditions in question 1, show that Eq. (1.15) dissipates entropy.
3. Adapt Stampacchia's method to prove L^∞ bounds on n_1, n_2 (and which is the appropriate quantity for the maximum principle). What are the intuitive L^p bounds.

Exercise Consider (1.15) with Dirichlet boundary conditions and $n_i^0 \ge 0$.

1. Using the inequality $\frac{\partial n_j}{\partial \nu} \leq 0$, which holds because $n_j \geq 0$, show that $M(t)$ decreases where

$$M(t) = \int_\Omega \big[2n_1(t,x) + n_2(t,x)\big]dx.$$

2. Consider the entropies of the previous exercise with the additional condition $\Sigma_i'(0) = 0$. Show Eq. (1.15) dissipates entropy.
3. Show that solutions of (1.15) with Dirichlet boundary conditions tend to 0 as $t \to \infty$.

2.4 Entropy: Chemostat and SI System of Epidemiology

Examples of entropy also appear in biological models. We treat here an example that arises as a first modeling stage in two applications: (1) ecology and the model of the chemostat (then u represents a nutrient, v a population that consumes the nutrient), (2) epidemiology with the celebrated Susceptible-Infected model (SI system). In both cases the model is

$$\begin{cases} \frac{d}{dt}u = B - \mu_u u - ruv, \\ \frac{d}{dt}v = ruv - \mu_v v, \end{cases} \tag{2.15}$$

with $B > 0$, $r > 0$, $\mu_u > 0$ and $\mu_v > 0$ parameters.

In the chemostat B represents the renewal of nutrients u, μ_u the removal or degradation of nutrients and r the consumption rate by the population and μ_v is the mortality and removal rate of the population.

In epidemiology, B represents the newborn, μ_u the mortality rate, r the encounter rate between susceptible and infected individuals (these encounters are responsible of new infected), μ_v is the mortality of the infected (and recovery rate in the SIR model).

There is always a trivial steady state

$$\bar{u}_0 = B/\mu_u, \qquad \bar{v}_0 = 0,$$

and a positive steady state

$$\bar{u} = \mu_v/r, \qquad \bar{v} = \frac{rB - \mu_u\mu_v}{r\mu_v} \qquad \text{if} \quad rB > \mu_u\mu_v. \tag{2.16}$$

Depending on the sign of $\bar{v}$ we may have two different Lyapunov functionals (entropies)

Lemma 2.4 *Defining*

$$\bar{S}(u,v) = -\bar{u}\ln(u) - \bar{v}\ln(v) + u + v,$$

we have

$$\frac{d}{dt}\bar{S} = -\frac{1}{u}(\sqrt{\bar{u}B} - u\sqrt{\bar{v}r + \mu_u})^2. \tag{2.17}$$

Lemma 2.5 *We assume $rB \le \mu_u\mu_v$ and define*

$$\underline{S}(u, v) = -\bar{u}_0 \ln(u) + u + v,$$

we have

$$\frac{d}{dt}\underline{S} = -\frac{v}{\mu_u}(\mu_v\mu_u - rB) - \frac{1}{\mu_u u}(B - \mu_u u)^2. \tag{2.18}$$

We leave the proofs of these lemmas to the reader and go directly to the conclusion

Proposition 2.6 *Solutions of the system* (2.15) *behave as follows*

If $Br > \mu_u\mu_v$, then the entropy $\bar{S}$ is convex and all solutions with $v^0 > 0$ converge as $t \to \infty$ to the positive steady state.

If $Br \le \mu_u\mu_v$, then solutions become extinct (they converge to the trivial steady state as $t \to \infty$).

The proof is standard and left to the reader. The steps are (i) $u(t)$ is bounded, (ii) $S(t)$ decreases, in the case $\bar{v} < 0$, the limit can be $-\infty$ and this means that $v(t)$ vanishes and the result (ii) follows, otherwise S stays bounded and converges to a finite value, (iii) we conclude thanks to the right hand side of (2.17).

2.5 The Spectral Decomposition of Laplace Operators

We have used consequences of the spectral decomposition of the Laplace operator with either a Dirichlet boundary condition

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{2.19}$$

or a Neumann boundary condition

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ \frac{\partial u}{\partial \nu} = 0 & \text{on } \partial\Omega, \end{cases} \tag{2.20}$$

2.5.1 Main Results

Theorem 2.7 (Dirichlet) *Consider a bounded connected open set Ω, then there is a spectral basis $(\lambda_k, w_k)_{k\geq 1}$ for (2.19), that is,*

(i) λ_k *is a non-decreasing sequence with* $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_k \leq \ldots$ *and* $\lambda_k \underset{k\to\infty}{\longrightarrow} \infty$,

(ii) (λ_k, w_k) *are eigenelements, i.e., for all* $k \geq 1$ *we have*

$$\begin{cases} -\Delta w_k = \lambda_k w_k \qquad \text{in } \Omega\,, \\ w_k = 0 \qquad \text{on } \partial\Omega\,, \end{cases}$$

(iii) $(w_k)_{k\geq 1}$ *is an orthonormal basis of* $L^2(\Omega)$,

(iv) we have $w_1(x) > 0$ *in* Ω *and the first eigenvalue* λ_1 *is simple, and for* $k \geq 2$, *the eigenfunction* w_k *changes sign and can be multiple.*

Theorem 2.8 (Neumann) *Consider a C^1 bounded connected open set Ω, then there is a spectral basis $(\lambda_k, w_k)_{k\geq 1}$ for (2.20), i.e.,*

(i) λ_k *is a non-decreasing sequence with* $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_k \leq \ldots$ *and* $\lambda_k \underset{k\to\infty}{\longrightarrow} \infty$,

(ii) (λ_k, w_k) *are eigenelements, i.e., for all* $k \geq 1$ *we have*

$$\begin{cases} -\Delta w_k = \lambda_k w_k \qquad \text{in } \Omega\,, \\ \frac{\partial w_k}{\partial \nu} = 0 \qquad \text{on } \partial\Omega\,, \end{cases}$$

(iii) $(w_k)_{k\geq 1}$ *is an orthonormal basis of* $L^2(\Omega)$

(iv) $w_1(x) = \frac{1}{|\Omega|^{1/2}} > 0$, *and for* $k \geq 2$, *the eigenfunction* w_k *changes sign.*

Remark 1 The hypothesis that Ω is connected is simply used to guarantee that the first eigenvalue is simple and the corresponding eigenfunction is positive in Ω. Otherwise, we have several additional nonnegative eigenfunctions with a first eigenfunction in one component and 0 in the others.

Remark 2 The sequences w_k are also orthogonal in $H_0^1(\Omega)$ (for Dirichlet boundary conditions) and $H^1(\Omega)$ for Neumann boundary conditions. Indeed, if w_k is orthogonal to w_j in $L^2(\Omega)$, then from the Laplace equation for w_k and the Stokes formula

$$\int_\Omega \nabla w_j \nabla w_k = \lambda_k \int_\Omega w_j w_k = 0.$$

Therefore, orthogonality in L^2 implies orthogonality in H_0^1 or H^1.

Note that for $k \geq 2$, the eigenfunction w_k changes sign because $\int_\Omega w_1 w_k = 0$ and w_1 has a sign.

Proof of Theorem 2.7 We only prove the first theorem, the second being a variant and we do not give the details. For additional matters see [3] Chap. 5, [1] p. 96. The result is based on two ingredients. (i) The spectral decomposition of self-adjoint compact linear mappings on Hilbert spaces is a general theory that extends the case of symmetric matrices. (ii) The simplicity of the first eigenvalue with a positive eigenfunction is also a consequence of the Krein-Rutman theorem (infinite dimension version of the Perron-Froebenius theorem).

First Step. First Eigenelements In the Hilbert space $H = L^2(\Omega)$, we consider the linear subspace $V = H_0^1(\Omega)$. Then we define the minimum on V

$$\lambda_1 = \min_{\int_\Omega |u|^2=1} \int_\Omega |\nabla u|^2 dx.$$

This minimum is achieved because a minimizing sequence (u_n) will converge strongly in H and weakly in V to $w_1 \in V$ with $\int_\Omega |w_1|^2 = 1$, by the Rellich compactness theorem (see [1, 2]). Therefore, $\int_\Omega |\nabla w_1|^2 dx \leq \liminf_{n\to\infty} \int_\Omega |\nabla u_n|^2 dx = \lambda_1$. This implies equality and that $\lambda_1 > 0$. The variational principle associated to this minimization problem says that

$$-\Delta w_1 = \lambda_1 w_1,$$

which implies that w_1 is smooth in Ω (by elliptic regularity).

Second Step. Positivity Because in V, $\left|\nabla |u|\right|^2 = |\nabla u|^2$ a.e., the construction above tells us that $|w_1|$ is also a first eigenfunction and we may assume that w_1 is nonnegative. By the strong maximum principle applied to the Laplace equation, we obtain that w_1 is positive inside Ω (because it is connected). This also proves that all the eigenfunctions associated with λ_1 have a sign in Ω because, in a connected open set, w_1 cannot satisfy the three properties (i) be smooth, (ii) change sign and (iii) $|w_1|$ be positive also.

Third Step. Simplicity Finally, we can deduce the simplicity of this eigenfunction because if there were two independent eigenfunction, a linear combination would allow us to build one which changes sign (by orthogonality to w_1 for example) and this is impossible by the above positivity argument.

Fourth Step. Other Eigenelements We may iterate the construction. Denote E_k the finite dimensional subspace generated by the k-th first eigenspaces. We work on the closed subspace $E_k^\perp$ of H, and we may define

$$\lambda_{k+1} = \min_{u \in E_k^\perp \cap V, \int_\Omega |u|^2=1} \int_\Omega |\nabla u|^2 dx.$$

This minimum is achieved by the same reason as before. The variational form gives that the minimizers are solutions of the $k+1$-th eigenproblem. They can form a multidimensional space but always finite dimensional; otherwise we would have an infinite dimensional subspace of $L^2(\Omega)$, whose unit ball is compact thanks to the Rellich compactness theorem, since $\int_\Omega |\nabla u|^2 dx \leq \lambda_{k+1}$ in this ball

Also $\lambda_k \to \infty$ as $k \to \infty$ because one can easily build (with oscillations or sharp gradients) functions satisfying $\int_\Omega |u_n|^2 = 1$ and $\int_\Omega |\nabla u_n|^2 dx \geq n$.

□

2.5.2 *Rectangles: Explicit Solutions*

In one dimension, one can compute explicitly the spectral basis because the solutions of $-u'' = \lambda u$ are all known. On $\Omega = (0, 1)$ we have

$$w_k = a_k \sin(k\pi x), \quad \lambda_k = (k\pi)^2, \qquad \text{(Dirichlet)}$$

$$w_k = b_k \cos\big((k-1)\pi x\big), \quad \lambda_k = \big((k-1)\pi\big)^2, \qquad \text{(Neumann)}$$

and a_k and b_k are normalization constants that ensure $\int_0^1 |w_k|^2 = 1$.

In two dimensions, on a rectangle $(0, L_1) \times (0, L_2)$ we see that the family is better described by two indices $k \geq 1$ and $l \geq 1$ and we have

$$w_{kl} = a_{kl} \sin(k\pi \frac{x_1}{L_1}) \sin(l\pi \frac{x_2}{L_2}), \qquad \lambda_{kl} = \big((\frac{k}{L_1})^2 + (\frac{l}{L_2})^2\big)\pi^2, \qquad \text{(Dirichlet)}$$

$$w_{kl} = b_{kl} \cos\big((k-1)\pi \frac{x}{L_1}\big) \cos\big((l-1)\pi \frac{x}{L_2}\big),$$

$$\lambda_{kl} = \big((\frac{k-1}{L_1})^2 + (\frac{l-1}{L_2})^2\big)\pi^2, \qquad \text{(Neumann)}$$

These examples indicate that

- The first positive eigenvalue is of the order of $1/\max(L_1, L_2)^2 = \frac{1}{\mathrm{diam}(\Omega)^2}$. For a large domain (even with a large aspect ratio) we can expect that the first eigenvalues are close to zero and that the eigenvalues are close to each other.
- Except the first one, eigenvalues can be multiple (take $L_1/L_2 \in \mathbb{N}$).
- Large eigenvalues are associated with highly oscillating eigenfunctions.

2.6 The Lotka-Volterra Prey-Predator System with Diffusion (Problem)

In the case of the Lotka-Volterra prey-predator system we can show relaxation towards a homogeneous solution. The coefficients of the model need not be small as is required in Theorem 2.2. This is because the model comes with a physically relevant quantity (such as entropy), which gives a global control.

Exercise Consider the prey-predator Lotka-Volterra system without diffusion

$$\begin{cases} \frac{\partial}{\partial t} n_1 = n_1[\ r_1 - a n_2], \\ \frac{\partial}{\partial t} n_2 = n_2[-r_2 + b n_1], \end{cases}$$

where r_1, r_2, a and b are positive constants and the initial data n_i^0 are positive.

1. Show that there are local solutions and that they remain positive.
2. Show that the entropy (Lyapunov functional)

$$E(t) = -r_1 \ln n_2 + a n_2 - r_2 \ln n_1 + b n_1,$$

   is constant. Show that E is bounded from below and that $E \to \infty$ as $n_1 + n_2 \to \infty$. Conclude that solutions are global.
3. What is the unique steady state solution?
4. Show, using question 2. that the solutions are periodic (trajectories are closed).

Solution

1. By local Lipschitz regularity of the right hand side, the Cauchy-Lipschitz theorem asserts that there is a *local* solution, i.e., defined on a maximal interval $[0, T^*]$. We can write

$$n_1(t) = n_1^0 e^{\int_0^t [r_1 - a n_2(s)] ds} > 0,$$

   and, same thing for n_2.
2. Set $\varphi_i = \ln n_i$ and write

$$\begin{cases} \frac{\partial}{\partial t} \varphi_1 = r_1 - a n_2 = r_1 - a e^{\varphi_2}, \\ \frac{\partial}{\partial t} \varphi_2 = -r_2 - b n_1 = -r_2 + b e^{\varphi_1}. \end{cases}$$

   This is a Hamiltonian system and the Hamiltonian is constant along trajectories

$$\mathcal{H}(t) = -r_1 \varphi_2(t) + a e^{\varphi_2(t)} - r_2 \varphi_1(t) + b e^{\varphi_1(t)} = \mathcal{H}(0).$$

   This proves that the $\varphi_i(t)$ remain bounded from above and below, and thus that solutions are global.
3. $\bar{n}_1 = r_2/b, \bar{n}_2 = r_1/a$.
4. In each quadrant defined by the origin $(\bar{n}_1, \bar{n}_2)$, we can write n_2 as a function of n_1 (or vice versa) and conclude from that.

□

Exercise Let Ω be a smooth bounded domain. Consider smooth positive solutions of the Lotka-Volterra equation with diffusion and a Neumann boundary condition

$$\begin{cases} \frac{\partial}{\partial t} n_1 - d_1 \Delta n_1 = n_1[\ r_1 - a n_2], \\ \frac{\partial}{\partial t} n_2 - d_2 \Delta n_2 = n_2[-r_2 + b n_1], \\ \frac{\partial n_i}{\partial \nu} = 0 \quad \text{on } \partial\Omega, \quad i = 1,\ 2, \end{cases}$$

where d_1, d_2, r_1, r_2, a and b are positive constants and the initial data n_i^0 are positive.

1. Consider the quantity $m(t) = \int_\Omega [b n_1(t,x) + a n_2(t,x)]dx$. Show that $m(t) \leq m(0)e^{rt}$ and find the value r.
2. Show that the convex entropy

$$E(t) = \int_\Omega [-r_1 \ln n_2 + a n_2 - r_2 \ln n_1 + b n_1] dx,$$

   a) is bounded from below, b) is decreasing.

   Conclude that $m(t)$ is bounded.
3. What finite integral do we obtain from the entropy dissipation?
3. Assume that the quantities $\nabla \ln n_i(t,x)$ converge, as $t \to \infty$,

   a. What are their limits?
   b. What can you conclude about the behavior of $n_i(t,x)$ as $t \to \infty$?

2.7 Problem

Let Ω a smooth bounded domain. Consider smooth positive solutions of the Lotka-Volterra system with diffusion and Neumann boundary condition

$$\begin{cases} \frac{\partial}{\partial t} n_i - D_i \Delta n_i + a_i(x) n_i = n_i\ r_i(t), \qquad t \geq 0,\ x \in \Omega, \quad i = 1,2,\dots,I, \\ \frac{\partial n_i}{\partial \nu} = 0 \quad \text{on } \partial\Omega, \quad i = 1,2,\dots,I, \\ n_i(t=0,x) = n_i^0(x), \end{cases}$$

with the nonlinearity defined, for some given functions $\big(\psi_i(x)\big)_{i=1,\dots,I}$, by

$$r_i(t) = \mathcal{R}_i\Big(\int_\Omega \psi_1(x) n_1(t,x)dx, \dots, \int_\Omega \psi_I(x) n_I(t,x)dx\Big).$$

1. We give real numbers λ_i. Show that the solution can be written as $n_i(t,x) = \rho_i(t)\tilde{n}_i(t,x)$ with $\tilde{n}_i$ the solution of

$$\begin{cases} \frac{\partial}{\partial t}\tilde{n}_i - D_i\Delta\tilde{n}_i + a_i(x)\tilde{n}_i = \lambda_i\tilde{n}_i, \qquad t \geq 0,\ x \in \Omega, \quad i = 1,2,\ldots,I, \\ \frac{\partial n_i}{\partial \nu} = 0 \quad \text{on } \partial\Omega, \quad i = 1,2,\ldots,I, \\ \tilde{n}_i(t=0,x) = n_i^0(x). \end{cases}$$

   Identify the evolution equation giving the $\rho_i(t)$ in terms of the $\tilde{n}_i$.
2. Assume that 0 is the first eigenvalue of the operator $u \mapsto D_i\Delta u + [a_i(x) - \lambda_i]$, associated with the positive eigenfunction $N_i(x)$, that $\tilde{n}(t,x) \to \alpha N(x)$ in all $L^p(\mathbb{R}^d)$ as $t \to 0$ (this is a standard consequence of the Krein-Rutman theorem) and that $\mathcal{R}(+\infty) < 0$ and $\mathcal{R}(-\infty) > 0$. Show that the long term dynamic is given by that of the equation

$$\dot{\varrho}(t) = \varrho(t)\ \mathcal{R}\big(\varrho(t)\alpha \int \psi(x)N(x)dx\big),$$

   and that $n(t,x)$ converges generically to a steady state $\bar{\rho}N(x)$ as $t \to \infty$.

References

1. Brezis, H.: Analyse Fonctionnelle, Théorie et Applications. Masson, Paris (1983)
2. Evans, L.C.: Partial Differential Equations. Graduate Studies in Mathematics, vol. 19. American Mathematical Society, Providence, RI (1998)
3. Gilbarg, D., Trudinger, N.: Elliptic Partial Differential Equations of Second Order, 2nd edn. Springer, Berlin (2003)
4. Jost, J.: Mathematical Methods in Biology and Neurobiology. Universitext. Springer (2014)

Chapter 3
Weak Solutions of Parabolic Equations in Whole Space

So far, we have manipulated parabolic equations in a formal way, integrating in the whole space and writing mass, entropy or energy equalities with the claim that solutions vanish at infinity. Here we introduce precisely what is the concept of weak solutions and justify these integrations by parts.

This chapter is solely of mathematical interest.

3.1 Weak Solutions in the Sense of Distributions

So far, our statements always concern weak solutions $u \in C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$ to parabolic equations of the type

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = f \qquad \text{in } \mathbb{R}^d, \\ u(t=0,x) = u^0(x). \end{cases} \tag{3.1}$$

According to the general theory of distributions, these are defined through a formal integration by parts against a test function $\Phi(t,x)$

Definition 3.1 Let $f \in L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^d)$, $u^0 \in L^1_{\text{loc}}(\mathbb{R}^d)$. A function $u \in L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^d)$ is a weak solution (or a distributional solution) of (3.1) if we have

$$\int_0^\infty \int_{\mathbb{R}^d} u(t,x)[-\frac{\partial \Phi}{\partial t} - \Delta\Phi]dx\, dt = \int_0^\infty \int_{\mathbb{R}^d} f(t,x)\Phi(t,x)dx\, dt + \int_{\mathbb{R}^d} u^0(x)\Phi(t=0,x)\, dx, \tag{3.2}$$

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_3

for all test functions $\Phi \in \mathcal{D}\big([0,+\infty)\times\mathbb{R}^d\big)$.[1] We can also consider locally bounded measures or derivatives of functions here.

In particular, when $u(t,x)$ is a C^2 function, this holds obviously true.

Variants of this definition are possible (all of them are equivalent and we show that later). When $u \in C(\mathbb{R}^+; L^1_{\mathrm{loc}}(\mathbb{R}^d))$, in place of (3.2), one can also use that for all $T \geq 0$

$$\int_{\mathbb{R}^d} u(T,x)\Phi(T,x)\,dx + \int_0^T \int_{\mathbb{R}^d} u(t,x)[-\frac{\partial \Phi}{\partial t} - \Delta\Phi]\,dx\,dt$$
$$= \int_0^\infty \int_{\mathbb{R}^d} f(t,x)\Phi(t,x)\,dx\,dt + \int_{\mathbb{R}^d} u^0(x)\Phi(t=0,x)\,dx. \tag{3.3}$$

This relation also holds when $u \in L^1_{\mathrm{loc}}(\mathbb{R}^+\times\mathbb{R}^d)$ at all Lebesgue points T of $\int_{\mathbb{R}^d} u(t,x)\Phi(t,x)\,dx$.

Weak solutions of linear equations enjoy many properties that justify the interest of this notion. This is the goal of this chapter to show that they can be manipulated as classical solutions.

3.2 Stability of Weak Solutions

The first useful property of weak solutions is that they are compatible with weak limits.

Consider a sequence of weak solutions u_n of (3.1) corresponding to data u_n^0 and f_n. Assume convergence in some weak topology (for example L^2, L^1, M^1 (measures))

$$u_n^0 \rightharpoonup u^0, \qquad f_n \rightharpoonup f, \qquad u_n \rightharpoonup u.$$

Then we have the

Lemma 3.2 *In this situation the limit u is a weak solution of* (3.1).

Proof By definition of weak solution, for a test function $\Phi \in \mathcal{D}\big([0,+\infty)\times\mathbb{R}^d\big)$ we have

$$\int_0^\infty \int_{\mathbb{R}^d} u_n(t,x)[-\frac{\partial \Phi}{\partial t} - \Delta\Phi]dx\,dt = \int_0^\infty \int_{\mathbb{R}^d} f_n(t,x)\Phi(t,x)$$
$$+ \int_{\mathbb{R}^d} u_n^0(x)\Phi(t=0,x)\,dx,$$

[1] $\mathcal{D}$ is the vector space of C^∞ functions with compact supports.

but Φ being fixed, and by the very definition of weak convergence, we can pass to the limit as $n \to \infty$ and recover the relation (3.2). $\square$

3.3 Mass Conservation and Truncation

Among the desirable properties of solutions is that the mass conservation law holds true. In other words we can integrate in the whole space and not bother with the 'boundary terms at infinity'. This is indeed true

Proposition 3.3 *Assume $u^0(x) \in L^1(\mathbb{R}^d)$, $f \in L^1([0,T] \times \mathbb{R}^d)$ for all $T > 0$. Let $u \in L^1([0,T] \times \mathbb{R}^d)$ for all $T > 0$ be a weak solution of (3.1), then $\int_{\mathbb{R}^d} u(t,x)dx \in C(\mathbb{R}^+)$ and*

$$\int_{\mathbb{R}^d} u(t,x)dx = \int_0^t \int_{\mathbb{R}^d} f(s,x)dx\, ds + \int_{\mathbb{R}^d} u^0(x)dx.$$

Another equivalent statement is that, in the weak sense,

$$\frac{d}{dt}\int_{\mathbb{R}^d} u(t,x)dx = \int_{\mathbb{R}^d} f(t,x)dx. \tag{3.4}$$

We point out that it is necessary and important that we know a priori that the functions u^0, f, u are integrable. For $f \equiv 0$, $u^0 \equiv 0$, there are non-zero solutions of the heat equation with a super-exponential growth at infinity.

Proof (Truncation Method) In Definition 3.1, we can use a test function $\chi_R(x)$ with

$$\begin{cases} \chi \in \mathcal{D}(\mathbb{R}^d), \qquad 0 \le \chi(\cdot) \le 1, \qquad \chi_R(x) = \chi(\frac{x}{R}), \\ \chi(x) = 1 \ \text{ for } \ |x| \le 1, \qquad \chi(x) = 0 \ \text{ for } \ |x| \ge 2. \end{cases} \tag{3.5}$$

We have for any test function $\phi \in \mathcal{D}(\mathbb{R}^+)$ and $\Phi(t,x) = \phi(t)\chi_R(x)$,

$$-\int_0^\infty \int_{\mathbb{R}^d} u(t,x)\chi_R(x)\phi'(t) = \int_0^\infty \int_{\mathbb{R}^d} \left[u(t,x)\Delta\chi_R(x) + f(t,x)\chi_R(x)\right]\phi(t) + \int_{\mathbb{R}^d} u^0(x)\chi_R(x)\phi(0).$$

Because $\Delta\chi_R(x) = \frac{1}{R^2}\Delta\chi(\frac{x}{R})$ and u, u^0 and f belong to $L^1([0,T) \times \mathbb{R}^d)$, we can let $R \to \infty$ and obtain, using the Lebesgue Dominated Convergence theorem, that

$$-\int_0^\infty \int_{\mathbb{R}^d} u(t,x)\phi'(t) = \int_0^\infty \int_{\mathbb{R}^d} f(t,x)\phi(t) + \int_{\mathbb{R}^d} u^0(x)\phi(0).$$

In other words, the functions defined as $M_u(t) = \int_{\mathbb{R}^d} u(t,x)dx$ and $M_f(t) = \int_{\mathbb{R}^d} f(t,x)dx$ are related through

$$-\int_0^\infty M_u(t)\phi'(t) = \int_0^\infty M_f(t)\phi(t) + \int_{\mathbb{R}^d} u^0(x)\phi(0). \tag{3.6}$$

This is the meaning of (3.4). However, because $M_u(t)$, $M_f(t)$ are simply $L^1_{loc}(\mathbb{R}^+)$ functions, we cannot derive immediately the integral form directly.

Proof of Mass Balance Equation Let $T > 0$, we would like to use the test function $\phi(t) = \mathbf{1}_{\{0 \le t \le T\}}$ in (3.6) and use that $\phi'(t) = -\delta(t-T)$.

It is not an admissible test function but we can choose a sequence of functions $\phi_n \in \mathcal{D}(\mathbb{R})$ with ϕ_n decreasing in t and increasing in n, $\phi_n(t) \le \phi(t)$ and $\phi_n(t) = 1$ in $[0, T - 1/n]$ (n large enough). Then we have from equality (3.6)

$$-\int_0^\infty M_u(t)\phi_n'(t) = \int_0^\infty M_f(t)\phi_n(t) + \int_{\mathbb{R}^d} u^0(x) \underset{n\to\infty}{\longrightarrow} \int_0^T M_f(t) + \int_{\mathbb{R}^d} u^0(x),$$

still by the Lebesgue Dominated Convergence theorem applied to M_f.

Because $-\phi_n'(t)$ can be chosen as any nonnegative approximation of $\delta(t-T)$, we deduce that M_u is continuous at T. Indeed, at each Lebesgue point T of M_u one can also pass to the limit in the left hand side of the above formula and obtain

$$M_u(T) = \int_0^T M_f(t)dt + \int_{\mathbb{R}^d} u^0(x).$$

This concludes the proof of the integral version of (3.4) and of Proposition 3.5. □

3.4 Regularization of Weak Solutions (Space)

The definition of weak solutions is by duality, a linear statement. However, several nonlinear properties of weak solutions can be derived from a regularization argument that we give now. It uses the regularization method

Definition 3.4 A regularizing kernel ω_ε, is a family of functions satisfying the properties

$$\omega_\varepsilon(x) = \frac{1}{\varepsilon^d}\,\omega(\frac{x}{\varepsilon}), \qquad \omega \in \mathcal{D}(\mathbb{R}^d), \qquad \omega \ge 0, \qquad \int_{\mathbb{R}^d} \omega = 1. \tag{3.7}$$

We regularize functions by convolution and set

$$u_\varepsilon(x) = \omega_\varepsilon * u(x) = \int_{\mathbb{R}^d} \omega_\varepsilon(x-y)u(y)dy = \int_{\mathbb{R}^d} \omega_\varepsilon(y)u(x-y)dy.$$

For $1 \le p \le \infty$ and $u \in L^p(\mathbb{R}^d)$, we have $\omega_\varepsilon * u \in C^\infty \cap L^p(\mathbb{R}^d)$ and

$$\|\omega_\varepsilon * u\|_{L^p(\mathbb{R}^d)} \le \int_{\mathbb{R}^d} \omega_\varepsilon(y)\|u(\cdot - y)\|_{L^p(\mathbb{R}^d)}dy = \|u\|_{L^p(\mathbb{R}^d)}.$$

More important is that for $1 \le p < \infty$, we have [1, 2]

$$\omega_\varepsilon * u \underset{\varepsilon\to 0}{\longrightarrow} u \qquad \text{in } L^p(\mathbb{R}^d).$$

Proposition 3.5 (Regularization of Weak Solutions) *Let ω_ε be a regularizing kernel, $f \in C\big(\mathbb{R}^+; L^1(\mathbb{R}^d)\big)$ and $u^0(x) \in L^1(\mathbb{R}^d)$. For a weak solution of (3.1), $u \in L^1([0,T] \times \mathbb{R}^d)$ $\forall T > 0$, then $\omega_\varepsilon * u$ belongs to $C^1\big(\mathbb{R}^+; C^2(\mathbb{R}^d)\big)$ and is a classical solution of (3.1) for a regularized right hand side $\omega_\varepsilon * f$ and initial data $\omega_\varepsilon * u^0$.*

Corollary 3.6 (Entropy Inequalities) *Consequently for any C^2, sublinear and convex function $S : \mathbb{R} \to \mathbb{R}$, we have, in the weak sense,*

$$\frac{\partial}{\partial t}S\big(u(t,x)\big) - \Delta S\big(u(t,x)\big) \le S'\big(u(t,x)\big)f(t,x),$$

and also

$$\int_{\mathbb{R}^d} S\big(u(t,x)\big)dx \le \int_0^t \int_{\mathbb{R}^d} S'\big(u(s,x)\big)f(s,x)dxds + \int_{\mathbb{R}^d} S\big(u^0(x)\big)dx, \qquad a.e.$$

$$\int_{\mathbb{R}^d} |u(t,x)|dx \le \int_0^t \int_{\mathbb{R}^d} |f(s,x)|dxds + \int_{\mathbb{R}^d} |u^0(x)|dx, \qquad a.e. \tag{3.8}$$

Proof of Proposition 3.5 We use the test function $\Phi(t,x) = \phi(t)\omega_\varepsilon(y-x)$ with a fixed vector $y \in \mathbb{R}^d$ and $\phi \in \mathcal{D}(\mathbb{R}^+)$ a given test function. For this choice, the Definition 3.2 gives

$$\int_0^\infty \left[-u(t) * \omega_\varepsilon(y)\frac{\partial\phi}{\partial t} - u(t) * \Delta\omega_\varepsilon(y)\phi(t)\right] dt$$
$$= \int_0^\infty f(t) * \omega_\varepsilon(y)\phi(t)dt + u^0 * \omega_\varepsilon(y)\phi(0).$$

We set $u_\varepsilon(t,x) = u * \omega_\varepsilon, f_\varepsilon(t,x) = f * \omega_\varepsilon$, these are two smooth functions in x and the above equality can also be written (changing the name of the variable from y to x)

$$\int_0^\infty \left[-u_\varepsilon(t,x)\frac{\partial\phi}{\partial t} - \Delta u_\varepsilon(t,x)\phi(t)\right] dt = \int_0^\infty f_\varepsilon(t,x)\phi(t)dt + u^0_\varepsilon(x)\phi(0).$$

We fix x and set $G = f_\varepsilon + \Delta u_\varepsilon \in L^1_{loc}(\mathbb{R}^+)$, and we rewrite the above equality as

$$-\int_0^\infty u_\varepsilon(t)\phi'(t)dt = \int_0^\infty G(t)\phi(t)dt + u^0_\varepsilon\phi(0),$$

for all test functions $\phi \in \mathcal{D}(\mathbb{R}^+)$. Then we first conclude that $u_\varepsilon \in C(\mathbb{R}^+)$ with the argument at the end of the proof of Proposition 3.3 (choosing $\phi_n \to \mathbf{1}_{\{0\le t\le T\}}$) and

$$u_\varepsilon(t,x) = \int_0^t G(s,x)ds + u^0_\varepsilon(x).$$

This proves that $\Delta u_\varepsilon \in C(\mathbb{R}^+)$ (because $\Delta u_\varepsilon = \Delta\omega_\varepsilon * u$ while $u_\varepsilon = \omega_\varepsilon * u$, and the argument also applies with $\Delta\omega_\varepsilon$ in place of ω_ε). Therefore, $G \in C(\mathbb{R}^+)$ and thus $u_\varepsilon \in C^1(\mathbb{R}^+)$.

□

Proof of Corollary 3.6 The proof is more involved because this inequality is a nonlinear statement. We still use the regularization argument and consider the $C^1_t C^2_x$ function $u_\varepsilon = u * \omega_\varepsilon$. It satisfies

$$\frac{\partial u_\varepsilon}{\partial t} - \Delta u_\varepsilon = f * \omega_\varepsilon.$$

We now use a function $S(\cdot) : \mathbb{R} \to [0,\infty)$ with the properties: it is smooth, it is a sublinear convex function, $S(0) = 0$ (see Fig. 3.1 for an example). Then, using the chain rule, we also have

$$\frac{\partial S(u_\varepsilon)}{\partial t} - \Delta S(u_\varepsilon) = -S''(u_\varepsilon)|\nabla u_\varepsilon|^2 + S'(u_\varepsilon)f * \omega_\varepsilon \le S'(u_\varepsilon)f * \omega_\varepsilon.$$

Because $S(u_\varepsilon) \in C\big(\mathbb{R}^+; L^1(\mathbb{R}^d)\big)$, we can use the truncation argument of Sect. 3.3 to integrate and find

$$\int_{\mathbb{R}^d} S\big(u_\varepsilon(t,x)\big)dx \le \int_0^t \int_{\mathbb{R}^d} S'\big(u_\varepsilon(s,x)\big)f(s,x)dxds + \int_{\mathbb{R}^d} S\big(u^0_\varepsilon(x)\big)dx.$$

As $\varepsilon \to 0$, we have $u_\varepsilon \to u$ and $S(u_\varepsilon) \to S(u)$ strongly in $L^1\big((0,T)\times\mathbb{R}^d\big)$, $\forall T > 0$. Therefore, we obtain the desired inequality

$$\int_{\mathbb{R}^d} S\big(u(t,x)\big)dx \le \int_0^t \int_{\mathbb{R}^d} S'\big(u(s,x)\big)f(s,x)dxds + \int_{\mathbb{R}^d} S\big(u^0(x)\big)dx. \tag{3.9}$$

In order to handle the singular case of the absolute value, we need more work. We may choose a family $S_\delta(\cdot)$ of smooth functions as above that regularizes the absolute

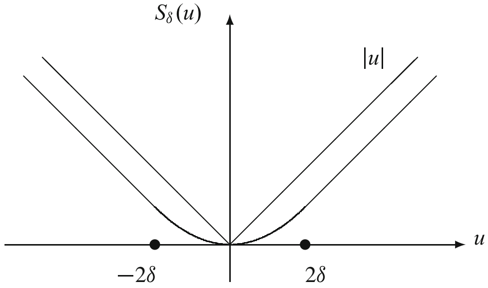

Fig. 3.1 The function $S_\delta(u)$ that regularizes $|u|$

value. The $S_\delta(\cdot)$ can fulfill the following properties (see Fig. 3.1 for an illustration):

$$\begin{cases} S_\delta(\cdot) \text{ is smooth, even and convex,} & \max(0, |u| - \delta) \leq S_\delta(u) \leq |u|, \\ 0 \leq \operatorname{sgn}(u) S'_\delta(u) \leq 1, & 0 \leq \frac{u}{2} S'_\delta(u) \leq S_\delta(u). \end{cases} \tag{3.10}$$

Then, (3.9) gives

$$\int_{\mathbb{R}^d} S_\delta\big(u(t,x)\big)dx \leq \int_0^t \int_{\mathbb{R}^d} |f(s,x)|dxds + \int_{\mathbb{R}^d} \big|u^0(x)\big|dx$$

and passing to the strong limit as $\delta \to 0$ we find the inequality (3.8). $\square$

Exercise Write and prove the same statement than those of Proposition 3.5 in $L^2(\mathbb{R}^d)$ in place of $L^1(\mathbb{R}^d)$ and in particular,

$$\|u(t)\|_{L^2(\mathbb{R}^d)} \leq \int_0^t \|f(s)\|_{L^2(\mathbb{R}^d)} ds + \|u^0\|_{L^2(\mathbb{R}^d)}.$$

3.5 Regularization of Weak Solutions (Time)

A direct way to relax the continuity assumptions in time is to use an additional regularization argument in time. To do so, there is a technical issue because $t \geq 0$ and we have to be careful when using convolution. This is the reason why we introduce an asymmetric regularizing kernel $\tilde{\omega}$, this is a function satisfying the properties

$$\tilde{\omega} \in \mathcal{D}(\mathbb{R}), \quad \tilde{\omega} \geq 0, \quad \tilde{\omega}(s) = 0 \text{ for } s \geq 0, \quad \int_{\mathbb{R}^d} \tilde{\omega} = 1. \tag{3.11}$$

Then, we can regularize a function $u(t) : \mathbb{R}^+ \to \mathbb{R}$ by convolution with the usual formula

$$\omega *_t u(t) = \int_{\mathbb{R}} \omega(t-s)u(s)ds.$$

It is well defined because we have $t - s \leq 0$ and thus for $t \geq 0$ we have $s \geq 0$.

Theorem 3.7 *Let $f \in L^1\big((0,T) \times \mathbb{R}^d\big)$ $\forall T > 0$, and $u^0(x) \in L^1(\mathbb{R}^d)$. For a weak solution of (3.1), $u \in L^1\big([0,T] \times \mathbb{R}^d\big)$ $\forall T > 0$, then $\big(\tilde{\omega}(t)\omega(x)\big) * u$ belongs to $C^1\big(\mathbb{R}^+; C^2(\mathbb{R}^d)\big)$ and is a classical solution of (3.1) for a regularized right hand side $\big(\tilde{\omega}(t)\omega(x)\big) * f$ and initial data $\omega * u^0$. Moreover*

$$\int_{\mathbb{R}^d} |u(t,x)|dx \leq \int_0^t \int_{\mathbb{R}^d} |f(s,x)|dxds + \int_{\mathbb{R}^d} |u^0(x)|dx \qquad a.e. \tag{3.12}$$

We simply write the main idea of the proof.

Proof We fix the space regularization kernel ω and use a regularizing kernel in time $\tilde{\omega}_\alpha = \frac{1}{\alpha}\tilde{\omega}(\frac{x}{\alpha})$. We define the smooth functions

$$U_\alpha(t,x) = \big(\tilde{\omega}_\alpha(t)\omega(x)\big) * u, \qquad F_\alpha(t,x) = \big(\tilde{\omega}_\alpha(t)\omega(x)\big) * f.$$

We use the test function $\Phi(s,y) = \tilde{\omega}_\alpha(t-s)\omega(x-y)$ in the definition of weak solutions of (3.1) written with the variables (s,y). Since $\tilde{\omega}_\alpha(t) = 0$ for $t \geq 0$, we find that the heat equation holds in the classical sense

$$\frac{\partial U_\alpha}{\partial t} - \Delta U_\alpha = F_\alpha, \qquad t \geq 0,\ x \in \mathbb{R}^d.$$

But the initial data is not recovered and we have to prove that

$$\|U_\alpha(0,x) - \omega * u^0(x)\|_{L^1(\mathbb{R}^d)} \underset{\alpha\to 0}{\longrightarrow} 0. \tag{3.13}$$

We use again the argument in Sect. 3.3, which proves that we may use the test function in time $\phi(s) = \mathbf{1}_{\{0\leq s\leq t\}}$ to find for all $x \in \mathbb{R}^d$

$$\omega * u(t,x) = \int_0^t [\Delta(\omega * u) + \omega * f](s,x)ds + \omega * u^0, \qquad a.e.\ t > 0,$$

and thus integrating in time with the weight $\tilde{\omega}(0-t)$, we find

$$U_\alpha(0,x) = \int \tilde{\omega}_\alpha(-t) \int_{s=0}^t [\Delta(\omega * u) + \omega * f](s,x)ds\ dt + \omega * u^0.$$

With $R_\alpha(s) = \int_s^\infty \tilde{\omega}_\alpha(-t)dt$, this can be written as

$$U_\alpha(0,x) - \omega * u^0(x) = \int_0^\infty R_\alpha(s)[\Delta(\omega * u) + \omega * f](s,x)ds \underset{\alpha\to 0}{\longrightarrow} 0, \qquad \forall x \in \mathbb{R}^d,$$

because $0 \le R_\alpha(s) \le 1$, $R_\alpha(s) \underset{\alpha\to 0}{\longrightarrow} 0$ a.e. in $(0,\infty)$. The result (3.13) follows because, choosing α sufficiently small, the support of R_α is less than a constant $C = O(\alpha)$ and

$$\left|\int_0^\infty R_\alpha(s)[\Delta(\omega * u) + \omega * f](s,x)ds\right| \le \int_0^C |\Delta(\omega * u) + \omega * f](s,x)|ds,$$

this is a fixed L^1 function, and we can apply the Lebesgue Dominated Convergence theorem.

In order to prove (3.12), we remark that this allows us to also recover the inequality

$$\int_{\mathbb{R}^d} S\big(U_\alpha(t,x)\big)dx \le \int_{s=0}^t \int_{\mathbb{R}^d} S'\big(U_\alpha(t,x)\big)F_\alpha(t,x)dx\, ds + \int_{\mathbb{R}^d} S\big(U_\alpha^0(x)\big)dx.$$

And in the limit $\alpha \to 0$, we obtain

$$\int_{\mathbb{R}^d} S\big(\omega * u(t,x)\big)dx \le \int_{s=0}^t \int_{\mathbb{R}^d} S'\big(\omega * u(t,x)\big)\ \omega * f(t,x)dx\, ds + \int_{\mathbb{R}^d} S\big(\omega * u^0(x)\big)dx.$$

We are back in the situation of Sect. 3.4, simply change ω in ω_ε. □

3.6 Uniqueness of Weak Solutions

Uniqueness is a direct consequence of the regularization method. Namely, we have the

Proposition 3.8 *Let $f \in L^1([0,T] \times \mathbb{R}^d)$ $\forall T > 0$, $u^0(x) \in L^1(\mathbb{R}^d)$ then there is at most one weak solution $u \in L^1([0,T] \times \mathbb{R}^d)$ $\forall T > 0$ of* (3.1).

Proof Indeed, subtracting two possible solutions u_1 and u_2, we find a solution of (3.1) with $f \equiv 0$, $u^0 \equiv 0$. Applying the inequality (3.12), we find

$$\int_{\mathbb{R}^d} |u_1(t,x) - u_2(t,x)|dx \le 0,$$

which implies that $u_1 = u_2$. □

3.7 Positivity of Weak Solutions of Lotka-Volterra Type Equations

The arguments of regularization and truncation are also useful to prove the positivity of weak solutions stated in Lemma 1.1, that is, we consider a weak solution $u \in C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$ to the parabolic equations

$$\begin{cases} \frac{\partial n}{\partial t} - \Delta n = nR(t,x) & \text{in } \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{3.14}$$

Then we have

Lemma 3.9 *Assume that the initial data n^0 is a nonnegative function in $L^2(\mathbb{R}^d)$ and that there is a locally bounded function $\Gamma(t)$ such that $|R(t,x)| \le \Gamma(t)$. Then, the weak solutions in $C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$ to the Lotka-Volterra system (1.1) satisfy $n(t,x) \ge 0$.*

Proof Again we are going to prove that the negative part vanishes following the method of Stampacchia. We set $p = -n$, $p_+ = \max(0,p)$ and we have to justify that the equation holds

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} \big(p(t,x)\big)_+^2 dx + \int_{\mathbb{R}^d} \left|\nabla (p)_+\right|^2 = \int_{\mathbb{R}^d} \big(p(t,x)\big)_+^2 R \le \Gamma(t)\int_{\mathbb{R}^d} \big(p(t,x)\big)_+^2. \tag{3.15}$$

To do so, we can regularize with a smoothing kernel $\omega_\varepsilon(\cdot)$ and write first

$$\frac{\partial}{\partial t}\omega_\varepsilon * p - \Delta\omega_\varepsilon * p = \omega_\varepsilon * (p\, R).$$

Then we handle a smooth function (C^∞ in x and C^1 in time if the R are continuous in time) as shown in Sect. 3.4. We can also use a truncation function $\chi_R(\cdot)$ as defined in (3.5). We obtain

$$\frac{\partial}{\partial t}\chi_R\omega_\varepsilon * p - \Delta[\chi_R\omega_\varepsilon * p] = \chi_R\omega_\varepsilon * (p\, R) - 2\nabla\chi_R\nabla\omega_\varepsilon * p - \omega_\varepsilon * p\Delta\chi_R.$$

Therefore, the chain rule indeed gives

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} \big(\chi_R\omega_\varepsilon * p(t,x)\big)_+^2 dx + \int_{\mathbb{R}^d} \left|\nabla(\chi_R\, \omega_\varepsilon * p)_+\right|^2 \\ &= \int_{\mathbb{R}^d} \big(\chi_R\omega_\varepsilon * p(t,x)\big)_+ \chi_R\omega_\varepsilon * (p\, R) \\ &\quad -2\int_{\mathbb{R}^d} \big(\chi_R\omega_\varepsilon * p(t,x)\big)_+ [\nabla\chi_R\nabla\omega_\varepsilon * p - \omega_\varepsilon * p\Delta\chi_R] dx \end{aligned}$$

and thus for $\delta > 0$

$$\tfrac{1}{2}\int_{\mathbb{R}^d} \big(\chi_R\omega_\varepsilon * p(t,x)\big)_+^2 dx \le \int_0^t \int_{\mathbb{R}^d} \big(\chi_R\omega_\varepsilon * p(s,x)\big)_+ \chi_R\omega_\varepsilon * (p(s)\; R(s))ds$$

$$+\delta \int_0^t \int_{\mathbb{R}^d} \big(\chi_R\omega_\varepsilon * p(t,x)\big)_+^2 + \tfrac{2}{\delta}\int_0^t \int_{\mathbb{R}^d} \big[|\nabla\chi_R \nabla\omega_\varepsilon * p|^2 + |\omega_\varepsilon * p\Delta\chi_R|^2\big]dx.$$

In the above expression, the last integral vanishes because $|\nabla\chi_R| \le C/R$ and $|\Delta\chi_R| \le C/R^2$ while $\nabla\omega_\varepsilon * p$ and $\omega_\varepsilon * p$ are L^2 functions because p is.

Therefore, using the Lebesgue Dominated Convergence theorem, we can pass to the limit at $R \to \infty$ and obtain

$$\frac{1}{2}\int_{\mathbb{R}^d} \big(\omega_\varepsilon * p(t,x)\big)_+^2 dx \le \int_0^t \int_{\mathbb{R}^d} \big(\omega_\varepsilon * p(s,x)\big)_+ \omega_\varepsilon * (p(s)\; R(s))ds$$
$$+\delta \int_0^t \int_{\mathbb{R}^d} \big(\omega_\varepsilon * p(s,x)\big)_+^2.$$

Then, we let $\varepsilon \to 0$ and obtain

$$\tfrac{1}{2}\int_{\mathbb{R}^d} \big(p(t,x)\big)_+^2 dx \le \int_0^t \int_{\mathbb{R}^d} \big(p(s,x)\big)_+ (p(s)\; R(s))ds + \delta\int_0^t \int_{\mathbb{R}^d} \big(p(s,x)\big)_+^2$$
$$\le \int_0^t [\Gamma(s)+1] \int_{\mathbb{R}^d} \big(p(s,x)\big)_+^2.$$

Because $\Gamma(t)$ is locally bounded the Gronwall lemma implies that $\int_{\mathbb{R}^d} \big(p(t,x)\big)_+^2 dx = 0$ and therefore, $p(t,x) \le 0$ almost everywhere.

Exercise Prove the same positivity result in L^1 in place of L^2.

Hint. replace $(u)_+^2$ by a convex function with linear growth at infinity.

3.8 Positivity of Weak Solutions of Reaction Kinetic Equations

In the same way, we consider a weak solution $u \in C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$ to the parabolic equations

$$\begin{cases} \frac{\partial n}{\partial t} - \Delta n + nR(t,x) = Q(t,x) \qquad \text{in } \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{3.16}$$

Lemma 3.10 *Assume* $|R(t,x)| \le \Gamma(t)$ *with* $\Gamma \in L^\infty_{\text{loc}}(\mathbb{R}^+)$ *and* $Q \in C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$. *If* $Q \ge 0$ *and* $n^0 \ge 0$, *then* $n \ge 0$.

We leave the proof as an exercise.

3.9 Heat Kernel and Explicit Solutions

3.9.1 Fundamental Solution

Before solving a nonlinear problem with (t, x) dependent coefficients as (3.16), it is usual (see [2, 4]) to look for the fundamental solution, which is called the heat kernel in the particular case of the heat equation. This is to solve the PDE with the initial data a Dirac mass, which is the problem

$$\begin{cases} \frac{\partial K}{\partial t} - \Delta K = 0 & \text{in } \mathbb{R}^d, \\ K(t = 0, x) = \delta(x). \end{cases} \tag{3.17}$$

Lemma 3.11 *The fundamental solution of the heat equation is given by the explicit form*

$$K(t, x) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}}. \tag{3.18}$$

This means that for all test functions $\Phi \in \mathcal{D}([0, T) \times \mathbb{R}^d)$ *there holds*

$$\int_0^T \int_{\mathbb{R}^d} K(t, x) \left[-\frac{\partial \Phi}{\partial t} - \Delta \Phi \right] dx\, dt = \Phi(t = 0, x = 0). \tag{3.19}$$

Notice that

$$\int_{\mathbb{R}^d} K(t, x) dx = 1 \qquad \forall t > 0, \tag{3.20}$$

$$K(\varepsilon, x) \rightharpoonup \delta(x) \qquad \text{as } \varepsilon \to 0^+ \qquad \text{in the weak sense of measures.} \tag{3.21}$$

Proof For $\varepsilon > 0$ sufficiently small, we have, by integration by parts,

$$\int_\varepsilon^T \int_{\mathbb{R}^d} K(t, x) \left[-\frac{\partial \Phi}{\partial t} - \Delta \Phi \right] dx\, dt$$
$$= \int_{\mathbb{R}^d} K(\varepsilon, x)\Phi(\varepsilon, x) dx + \int_\varepsilon^T \int_{\mathbb{R}^d} \left[\frac{\partial K}{\partial t} - \Delta K \right] \Phi$$

and one readily checks that $\frac{\partial K}{\partial t} - \Delta K = 0$ for $t > 0$ (left as an exercise). Therefore, we arrive at

$$\int_0^T \int_{\mathbb{R}^d} K(t, x) \left[-\frac{\partial \Phi}{\partial t} - \Delta \Phi \right] dx\, dt = \int_{\mathbb{R}^d} K(\varepsilon, x)\Phi(\varepsilon, x) dx$$
$$+ \int_0^\varepsilon \int_{\mathbb{R}^d} K(t, x) \left[-\frac{\partial \Phi}{\partial t} - \Delta \Phi \right] dx\, dt.$$

As $\varepsilon \to 0$, we obtain (3.19) because we may use (3.21) to pass to the limit in the first term in the right hand side and we may use (3.20) to bound

$$\int_0^\varepsilon \int_{\mathbb{R}^d} K(t,x) \left| -\frac{\partial \Phi}{\partial t} - \Delta \Phi \right| dx\, dt \leq \int_0^\varepsilon \sup_x \left| -\frac{\partial \Phi}{\partial t} - \Delta \Phi \right| dt \leq C\varepsilon.$$

□

Once the fundamental solution is known, one can also solve the Cauchy problem

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = 0 & \text{in } \mathbb{R}^d, \\ u(t=0,x) = u^0(x) \in L^p(\mathbb{R}^d). \end{cases}$$

Its solution is given by the convolution

$$u(t,x) = u^0 \star K(t) = \int_{\mathbb{R}^d} u^0(y) K(t,x-y) dy \in C\left(\mathbb{R}^+; L^p(\mathbb{R}^d)\right), \qquad 1 \leq p < \infty, \tag{3.22}$$

and for $p = \infty$ one has $u \in L^\infty(\mathbb{R}^+ \times \mathbb{R}^d)$.

When u^0 is smooth with sub-exponential growth (so as to be able to integrate in the convolution formula), this formula still makes sense and it is the smooth solution of the heat equation (but we only consider cases with integrability here).

3.9.2 *Time Decay*

For $u^0 \in L^p(\mathbb{R}^d)$, $1 \leq p \leq \infty$, this formula defines a function $u \in C^\infty((0,\infty)\times\mathbb{R}^d)$, which is the solution of the heat equation. Because we work in the full space the solution spreads, and thus decays when it is measured in the appropriate norms (not L^1!)

Lemma 3.12 (Decay Estimates) *The solution of the equation satisfies*

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \leq \|u^0\|_{L^p(\mathbb{R}^d)} \qquad \int_{\mathbb{R}^d)} u(t,x)dx = \int_{\mathbb{R}^d)} u^0(x)dx, \tag{3.23}$$

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \leq C(d,p)\, t^{-d/(2p')}\, \|u^0\|_{L^1(\mathbb{R}^d)}, \qquad \frac{1}{p'} = 1 - \frac{1}{p}. \tag{3.24}$$

An interesting conclusion is that the higher the norm under consideration, the faster is the time decay.

Proof Using convolution inequalities, we have, thanks to (3.20),

$$\|u(t)\|_{L^p(\mathbb{R}^d)} = \|u^0 \star K(t)\|_{L^p(\mathbb{R}^d)} \leq \|u^0\|_{L^p(\mathbb{R}^d)} \|K(t)\|_{L^1(\mathbb{R}^d)} = \|u^0\|_{L^p(\mathbb{R}^d)},$$

which proves the first result of (3.23). The second one follows, for $u^0 \in L^1(\mathbb{R}^d)$, from

$$\int_{\mathbb{R}^d} u(t,x)dx = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} u^0(y)K(t,x-y)dydx = \int_{\mathbb{R}^d} u^0(y)dy.$$

We also have

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \leq \|u^0\|_{L^1(\mathbb{R}^d)} \|K(t)\|_{L^p(\mathbb{R}^d)},$$

and

$$\|K(t)\|^p_{L^p(\mathbb{R}^d)} = \frac{1}{(2\pi t)^{pd/2}} \int_{R^d} e^{-p|x|^2/(2t)} dx = \frac{(2\pi t/p)^{d/2}}{(2\pi t)^{pd/2}},$$

$$\|K(t)\|_{L^p(\mathbb{R}^d)} \leq C(d,p) t^{\frac{d}{2}(\frac{1}{p}-1)}.$$

This gives (3.24), but with a constant which is not optimal despite the simplicity of the argument. □

A phenomena that is related to these decay estimates is diffusion. Consider $u^0 \geq 0$ and thus $u(t,x) \geq 0$ because $K(t,y) > 0$. Then we have

$$\int_{\mathbb{R}^d} u(t,x) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} u^0(x-y)K(t,y)dy\, dx = \int_{\mathbb{R}^d} u^0(x)dx := M,$$

and this equality is a special case of (3.4). But we also have

$$\begin{aligned}\int_{\mathbb{R}^d} |x|^2 u(t,x) &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} u^0(x-y)K(t,y)(|x-y|^2 - 2(x-y,y) + |y|^2)dy\, dx \\ &= \int_{\mathbb{R}^d} |x|^2 u^0(x)dx + M\int_{\mathbb{R}^d} |y|^2 K(t,y)dy \\ &= \int_{\mathbb{R}^d} |x|^2 u^0(x)dx + dMt,\end{aligned}$$

and using the truncation argument, this equality is also obtained directly in multiplying the heat equation by $|x|^2$ and integrating over $\mathbb{R}^d$.

The interpretation, together with the examples of Chap. 1, is as follows. Having in mind that individuals move randomly, their number is fixed, but they scatter further and further away from their initial position. The evaluation of the diffusion coefficient is often based on the measure of the second moment of the distribution: if it grows linearly in time, this is a sign of a normal diffusion and the slope gives the diffusion coefficient.

3.9.3 Right Hand Sides

Consequently, one can also find the solution of the inhomogeneous equation

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(t,x) & \text{in } \mathbb{R}^d, \\ u(t=0,x) = u^0(x). \end{cases} \tag{3.25}$$

It is simply given by the Duhamel formula

$$\begin{aligned} u(t,x) &= \int_0^t \int_{\mathbb{R}^d} K(t-s, x-y) Q(s,y) dy\, ds + K * u^0(x) \\ &= \int_0^t \int_{\mathbb{R}^d} K(t-s, y) Q(s, x-y) dy\, ds + K * u^0(x). \end{aligned}$$

An equivalent statement is that $J(t,x) = \int_0^t K(t-s,x)ds$ satisfies (left as an exercise)

$$\begin{cases} \frac{\partial J}{\partial t} - \Delta J = \delta(x) & \text{in } \mathbb{R}^d, \\ J(t=0,x) = 0. \end{cases}$$

The simplest a priori bounds for the solutions of (3.25) are now written (because the integral of a norm is less than the norm of the integral)

$$\begin{aligned} \|u(t)\|_{L^p(\mathbb{R}^d)} \leq \int_0^t \int_{\mathbb{R}^d} K(t-s,y) \|Q(s,\cdot - y)\|_{L^p(\mathbb{R}^d)} dy\, ds \\ + \int_{\mathbb{R}^d} K(t,y) \|u^0(\cdot - y)\|_{L^p(\mathbb{R}^d)} dy \end{aligned}$$

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \leq \int_0^t \|Q(s)\|_{L^p(\mathbb{R}^d)}\, ds + \|u^0\|_{L^p(\mathbb{R}^d)}, \tag{3.26}$$

still using the integral of K in (3.20).

Exercise Show that

1. for $Q \in L^1([0,T] \times \mathbb{R}^d)$, we have $\int_{\mathbb{R}^d} u(t,x)dx = \int_0^t Q(s,y)dy\, ds$,
2. for $Q \in L^1([0,T]; L^p(\mathbb{R}^d))$, we have

2a. $\|u(t)\|_{L^p(\mathbb{R}^d)} \leq \int_0^t \|Q(s)\|_{L^p(\mathbb{R}^d)} ds$, for all $p \in [1, \infty)$,

2b. $u \in C\big([0,T]; L^p(\mathbb{R}^d)\big)$ for all $1 \leq p < \infty$.

3. For $Q \in L^1([0,T]; L^\infty(\mathbb{R}^d))$, we have $u \in L^\infty([0,T] \times \mathbb{R}^d)$.

3.10 Nonlinear Problems

We present some examples of semilinear equations (the right hand side is nonlinear) and, for problems where nonlinearities arise in higher order terms, we refer to [2, 3, 5] and the references therein.

3.10.1 A General Result for Lipschitz Nonlinearities

The most standard existence theory consists of Lipschitz continuous nonlinearities in $L^p(\mathbb{R}^d)$, with $1 \le p < \infty$,

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(x, [u(t)]) & \text{in } \mathbb{R}^d, \\ u(t=0, x) = u^0(x) \in L^p(\mathbb{R}^d). \end{cases} \tag{3.27}$$

With this notation $Q(x, [u(t)])$ we mean that Q might depend in a non-local way (in x) on $u(t, x)$ and examples are given later.

To begin, we make two assumptions

$$\|Q(x, [u])\|_{L^p(\mathbb{R}^d)} \le M_Q \|u\|_{L^p(\mathbb{R}^d)}, \tag{3.28}$$

$$\|Q(x, [u]) - Q(x, [v])\|_{L^p(\mathbb{R}^d)} \le L_Q \|u - v\|_{L^p(\mathbb{R}^d)}. \tag{3.29}$$

Theorem 3.13 (Global Existence for the Nonlinear Heat Equation) *With the assumptions* (3.28)–(3.29) *and* $u^0(x) \in L^p(\mathbb{R}^d)$ *with* $1 \le p < \infty$, *then there is a unique weak solution* $u \in C(\mathbb{R}^+; L^p(\mathbb{R}^d))$ *of* (3.27)*.*

Proof We follow the standard proof of the Cauchy-Lipschitz theorem and consider a small T (to be chosen later), the Banach space $E = C\big([0, T]; L^p(\mathbb{R}^d)\big)$ and the mapping $\Phi : E \to E$ defined by $u = \Phi(v)$ is the solution of the equation of the type (3.25)

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(x, [v(t)]) & \text{in } \mathbb{R}^d,\ 0 \le t \le T, \\ u(t=0, x) = u^0(x) \in L^p(\mathbb{R}^d). \end{cases} \tag{3.30}$$

Notice that $u \in E$ because of assumption (3.28) and estimate (3.26).

We claim that for T sufficiently small, Φ is a strong contraction because

$$\|\Phi(v_1) - \Phi(v_2)\|_E \le L_Q T \|v_1 - v_2\|_E.$$

Indeed, from the property (3.26) of the solutions of (3.25) we have, using assumption (3.29),

$$\|u_1(t) - u_2(t)\|_{L^p(\mathbb{R}^d)} \le \int_0^t \|Q(s,[v_1(s)]) - Q(s,[v_2(s)])\|_{L^p(\mathbb{R}^d)} ds$$
$$\le L_Q \int_0^t \|v_1(s) - v_2(s)\|_{L^p(\mathbb{R}^d)} ds,$$

and thus

$$\|u_1 - u_2\|_E \le L_Q T \|v_1 - v_2\|_E.$$

Now choose T such that $L_Q T = 1/2$. The Banach-Picard fixed point theorem asserts there is a unique fixed point u. This is the unique solution of (3.27) in $[0,T]$.

We can iterate the argument to build a solution in $[T, 2T]$, $[2T, 3T]$, etc. □

3.10.2 Example 1

Consider the local nonlinear problem

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(u), \\ u(t=0,x) = u^0(x) \in L^p(\mathbb{R}^d), \qquad 1 \le p < \infty, \end{cases} \tag{3.31}$$

with

$$Q(0) = 0, \qquad |Q'(\cdot)| \le L_Q \qquad (\text{and thus } |Q(u)| \le L_Q |u|). \tag{3.32}$$

Corollary 3.14 *With assumption* (3.32)*, there is a unique solution of* (3.31) *in* $C\big([0,T]; L^p(\mathbb{R}^d)\big)$*. If, in addition,* $u^0 \in L^\infty(\mathbb{R}^d)$*, then*

$$\|u(t)\|_{L^\infty(\mathbb{R}^d)} \le \|u^0\|_{L^\infty(\mathbb{R}^d)} e^{L_Q t}.$$

Proof For the first statement, we can apply Theorem 3.13 because both assumptions (3.28) and (3.29) are satisfied (the details are left to the reader).

For the L^∞ bound, we use that $u(t,x) = K * u^0(x) + \int_0^t \int_{\mathbb{R}^d} K(t-s,y) Q(u)(s,x-y) dy\, ds$, then

$$\|u(t)\|_{L^\infty(\mathbb{R}^d)} \le \|u^0\|_{L^\infty(\mathbb{R}^d)} + \int_0^t \|Q(u(s))\|_{L^\infty(\mathbb{R}^d)}\, d \le \|u^0\|_{L^\infty(\mathbb{R}^d)}$$
$$+ L_Q \int_0^t \|u(s)\|_{L^\infty(\mathbb{R}^d)}\, ds.$$

We conclude thanks to the Gronwall lemma. □

Notice that, when $u^0 \in L^1 \cap L^\infty(\mathbb{R}^d)$, we obtain the same solution in all L^p. This can be seen from the construction by Picard iterations of the fixed point in Theorem 3.13. The uniqueness of the weak solution u for a given $Q(v)$ shows that the Picard iterations are the same for all L^p.

3.10.3 Example 2

Consider now the Fisher/KPP equation

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = u(1-u), \\ u(t=0,x) = u^0(x) \qquad \text{with } 0 \le u^0 \le 1, \quad u^0 \in L^1 \cap L^\infty(\mathbb{R}^d). \end{cases} \tag{3.33}$$

Theorem 3.13 cannot be applied directly because $u \mapsto u(1-u)$ is not Lipschitz continuous on $\mathbb{R}$. Nevertheless, based on a priori bounds, a small variant leads to the

Corollary 3.15 *There is a unique solution of* (3.33)*,* $u \in C\left(\mathbb{R}^+; L^p(\mathbb{R}^d)\right)$*,* $1 \le p < \infty$ *with*

$$0 \le u(t,x) \le 1.$$

Proof Define $Q(u) = \min(1,u_+)(1-u)$. This a Lipschitz continuous function vanishing at 0 and there is a solution of (3.31) with this right hand side thanks to Corollary 3.14.

The solution is nonnegative because we can write $Q(u) = uR(u)$ (left as exercise) and we can apply the positivity result of Sect. 3.7 and $u \ge 0$.

The solution is less than 1 because $v = 1-u$ satisfies

$$\begin{cases} \frac{\partial v}{\partial t} - \Delta v = -v \min(1,u), \\ v(t=0,x) = 1 - u^0(x) \ge 0. \end{cases}$$

Again from Sect. 3.7, v is nonnegative, which means that $u \le 1$.

Therefore, for the solution we also have $Q(u) = u(1-u)$ and the result is proved. □

3.10.4 Example 3

Consider the nonlocal Fisher/KPP equation

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = u(1-M*u), \\ u(t=0,x) = u^0(x) \qquad \text{with } u^0 \ge 0, \quad u^0 \in L^1 \cap L^\infty(\mathbb{R}^d). \end{cases} \tag{3.34}$$

Here we assume that

$$M \in L^1 \cap L^\infty(\mathbb{R}^d), \qquad M \geq 0, \qquad \int_{\mathbb{R}^d} M = 1. \tag{3.35}$$

Again we cannot apply directly Theorem 3.13 because of the quadratic aspect of the nonlinearity. Nevertheless a variant holds

Corollary 3.16 *With the assumption* (3.35)*, there is a unique solution of* (3.34)*, $u \in C\left(\mathbb{R}^+; L^p(\mathbb{R}^d)\right)$, $1 \leq p < \infty$ with*

$$0 \leq u(t,x) \leq \|u^0\|_{L^\infty(\mathbb{R}^d)} e^t.$$

And the bound $u \leq 1$ is lost for this nonlinear problem, which makes it interesting and its ability to create localized patterns as we see it later.

Proof We fix T and prove the result for the time interval $(0,T)$. We define

$$Q([u]) = \min(\|u^0\|_{L^\infty(\mathbb{R}^d)} e^T, u_+)\ (1 - M * u).$$

As in Example 2, Q being Lipschitz in L^p, there is a solution with the right hand side Q (it is global but we consider it only in the time interval $(0,T)$). Because we can write $Q(u) = uR(u)$ we have $u \geq 0$. Thus, $Q(u) \leq u$ and we can apply the L^∞ bound developed for (3.25) and find $0 \leq u(t,x) \leq \|u^0\|_{L^\infty(\mathbb{R}^d)} e^t$. Therefore, $Q(u) = u(1 - M * u)$ and we have in fact solved Eq. (3.35) in $(0,T)$ for all $T > 0$. □

References

1. Brezis, H.: Analyse Fonctionnelle, Théorie et Applications. Masson, Paris (1983)
2. Evans, L.C.: Partial Differential Equations. Graduate Studies in Mathematics, vol. 19. American Mathematical Society, Providence, RI (1998)
3. Quittner, P., Souplet, P.: Superlinear Parabolic Problems. Blow-Up, Global Existence and Steady State. Birkhäuser Advanced Texts. Birkhäuser, Basel (2007)
4. Schwartz, L.: Méthodes Mathématiques Pour les Sciences Physiques. Hermann, Paris (1983)
5. Vázquez, J.L.: The Porous Medium Equation: Mathematical Theory. Oxford Mathematical Monographs. The Clarendon Press, Oxford University Press, Oxford (2007). ISBN: 978-0-19-856903-9

Chapter 4
Traveling Waves

The relaxation results in Chap. 2 show that in bounded domains and with small nonlinearities we cannot expect spectacular behavior for solutions of reaction-diffusion equations. The situation is different when working in the whole space and, whatever the size of the nonlinearity, one can observe a first possible type of interesting behavior: *traveling waves*.

This chapter gives several examples motivated by models from biology even though combustion waves [32] or phase transitions (Allen-Cahn equation) are among the most famous examples of traveling waves. Historically, in 1930 Fisher [15] described the first model of wave propagation for a genetic advantage. But Kolmorov, Petrovski and Piskunov, [21], in 1937, presented the first mathematical analysis.

In biology, the name of Fisher [15] is associated with genetic invasion fronts. Traveling waves can also be epidemic spreads, such as bubonic plague in Europe in the fourteenth century (see Fig. 4.1). An example in neuroscience is calcium pulses propagating along a nerve, and these motivated J. Evans to introduce the so-called *Evans function* [13] for studying their stability. In ecology, traveling waves can describe the progress of an invasive species in an uncolonized environment. Moreover, experimental measurements also confirm that an invasion front moves approximately with constant speed, as predicted by reaction-diffusion equations. J.G. Skellam [30] reached the same conclusion by fitting to a linear distribution, the square root of the area occupied by muskrats, a North American species that escaped from a farm near Prague, see Fig. 4.1.

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_4

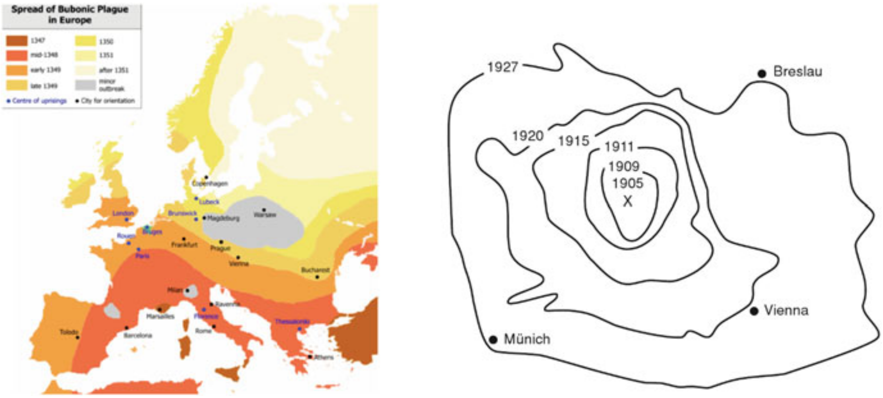

Fig. 4.1 *Left*: propagation of plague through Europe in the middle of the fourteenth century. *Source*: http://commons.wikimedia.org/wiki/File:Bubonic_plague_map.png. *Right*: spread of muskrats in the Czech Republic after J. G. Skellam and Ch. Elton. Reprinted from A. Okubo and P. Kareiva, Chap. 6 "Some examples of animal diffusion" in [28]

4.1 Setting the Problem

The simplest example is to consider the single equation

$$\frac{\partial}{\partial t}u - \frac{\partial^2}{\partial x^2}u = f(u), \qquad t \geq 0, \; x \in \mathbb{R}, \tag{4.1}$$

where $f(u)$ denotes a reaction term and $u(t,x) \in \mathbb{R}^+$ is the solution. It is usual that $f(u)$ allows two constant stationary states, say $f(0) = f(1) = 0$.

A first example is the so-called monostable equation (also called the Fisher/KPP equation) when

$$f(u) = u(1-u)$$

A simple observation is as follows: the steady state $u \equiv 0$ is unconditionally unstable. This means that any homogeneous small initial perturbation δu^0 will give, for short times, an exponential growth $u \approx e^{rt}\delta u^0$. But the steady state $u \equiv 1$ is unconditionally stable; for any homogeneous small initial perturbation $u^0 \approx 1$, the solution will relax exponentially to 1. These are the reasons why we expect that the 'colonized' state $u = 1$ invades the 'uncolonized' sate $u = 0$. To describe this invasion process, we look for solution $u(t,x) = v(x-ct)$.

Definition 4.1 A traveling wave solution is a solution of the form $u(t,x) = v(x-ct)$ with $c \in \mathbb{R}$ a constant called the *wave speed* or the *traveling speed*. We say it connects the states 1 and 0 if $v(-\infty) = 1$, $v(\infty) = 0$. See Fig. 4.2 for the example of Fisher/KPP wave.

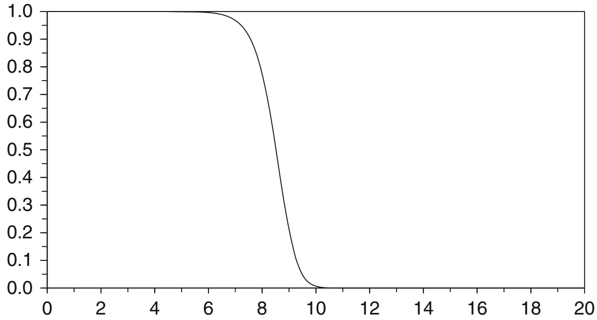

Fig. 4.2 Traveling wave solution to the Fisher/KPP equation (4.28) in the physical space. Abscissae x, ordinates $u(x)$

This definition can be applied to a wide range of nonlinearities f and to systems. A second example is the bistable equation (also called the Allen-Cahn equation)

$$f(u) = u(1-u)(u-\theta), \qquad 0 < \theta < 1.$$

When $c > 0$, this expresses that state $v = 1$ invades state $v = 0$ and vice-versa.

From Definition 4.1, we arrive at a simple equation, which determines both the wave speed c and the wave profile v

$$\begin{cases} -v''(x) - cv'(x) = f\big(v(x)\big), & x \in \mathbb{R}, \\ v(-\infty) = 1, \qquad v(+\infty) = 0. \end{cases} \tag{4.2}$$

Notice that this problem is translational invariant that means that, for all $a \in \mathbb{R}$, $v(x + a)$ is also a solution. Therefore, we can, for example, normalize it with $v(0) = \frac{1}{2}$.

There are two useful general observations. The first consists in integrating over the line and, because we expect that $v'(-\infty) = v'(\infty) = 0$ (or at least we can find two sequences $x_n^{\pm} \to \pm\infty$, where we can apply the reasoning), we find

$$c = \int_{-\infty}^{\infty} f\big(v(x)\big)dx. \tag{4.3}$$

The second observation is to compute the energy of the system

$$\frac{1}{2}\big(v'(x)^2\big)' + c\big(v'(x)^2\big) + \frac{d}{dx}F\big(v(x)\big) = 0.$$

with

$$F(u) = \int_0^u f(v)dv.$$

Because $v'(-\infty) = v'(\infty) = 0$, we find

$$c \int_{-\infty}^{\infty} v'(x)^2 dx = F(1) = \int_0^1 f(v)dv. \tag{4.4}$$

For example in the monostable case (Fisher/KPP equation) and for solutions such as $0 < v(x) < 1, f(\cdot) \geq 0$, these two equalities tell us that $c > 0$. This means that the state $v = 1$ is indeed invading. For the bistable case, we conclude from (4.4) that the sign of c depends on the value θ.

Exercise Show the additional relation

$$\int_{-\infty}^{\infty} v'(x)^2 dx = \int_{-\infty}^{\infty} \big(v(x) - \frac{1}{2}\big) f(v)dv.$$

A question comes now, which is to know what properties of the steady states imply that one can connect them by a traveling wave. Many examples [8, 10, 14, 31] are treated in the literature and cover the cases

- 0 is dynamically unstable ($f'(0) > 0$) and 1 is stable ($f'(1) < 0$); this is the case in the monostable equation (Fisher/KPP equation),
- 0 and 1 are dynamically stable ($f'(0) < 0, f'(1) < 0$); this is the bistable case,
- the state 0 is dynamically unstable and 1 is Turing unstable (see Chap. 7) and they can be connected by an unstable traveling wave. The example of the non-local Fisher/KPP equation is treated in G. Nadin et al. [27]
- the state 0 is connected to itself by a special traveling wave called a *pulse* (homoclinic orbits), this is typical of the FitzHugh-Nagumo and Hodgkin-Huxley systems (electric pulse propagation along the axon), see [17].

We first give the simplest results when there is a unique pair (c^*, v) that satisfies Eq. (4.2). This is the case both for the Fisher/KPP equation with ignition temperature and for the bistable equation. Then we turn to the more complicated case of the monostable equation (Fisher/KPP equation), where there is an infinity of traveling speeds, and finally we treat coupled systems of equations.

We begin with examples where the traveling wave can be computed analytically.

4.2 Analytical Example: The Fisher/KPP Equation with Ignition Temperature

For $\theta \in (0, 1)$, $\mu > 0$, consider the discontinuous function

$$f(u) = \begin{cases} 0 & \text{for } 0 \leq u < \theta, \\ \mu(1-u) & \text{for } \theta < u \leq 1. \end{cases} \tag{4.5}$$

We refer to Sect. 4.6 for the explanation of the terminology 'ignition temperature' for this case.

Lemma 4.2 *For f given by (4.5), there is a unique solution (c^*, v) of (4.2) such that v is decreasing and normalized with $v(0) = \theta$.*

Proof We know from (4.3), (4.4) that c should be positive. Thanks to the normalization and because we look for a decreasing solution, for $x < 0$ we look for a solution with $v > \theta$ and the equation reads $cv' + v'' + \mu(1-v) = 0$. The solutions are all of the form $v = 1 - w$ with $cw' + w'' - \mu w = 0$ and thus w is a linear combination of two exponential functions. Hence, we simply consider the characteristic polynomial, that is, $\lambda^2 + c\lambda - \mu = 0$. It has two roots of which only one is positive. Therefore, the solution which is decaying to zero at $-\infty$, is given by

$$v = 1 - (1-\theta)e^{\lambda_+ x}, \; x \leq 0, \qquad \lambda_+ = \lambda_+(c) := \frac{1}{2}[-c + \sqrt{c^2 + 4\mu}\,] > 0.$$

For $x > 0$ we look for $v < \theta$ and the equation is $cv' + v'' = 0$, which again has a single decaying solution, namely

$$v = \theta e^{-cx}, \quad x \geq 0.$$

It remains to check that v is differentiable at $x = 0$ (and v'' has a jump at 0 because of the discontinuity of f at θ), that is

$$(1-\theta)\lambda_+ = \theta c.$$

Because $2\frac{d}{dc}\lambda_+(c) = -1 + \frac{c}{\sqrt{c^2+4\mu}} < 0$, there is indeed a unique solution c^* to this equation. The explicit formulas show that v is decreasing. □

The traveling speed c^* results from a combination of the solution behind and in front of the transition point $x = 0$. For that reason it is called a pushed front.

Exercise Prove that a solution which satisfies $v \in (0, 1)$ is also decreasing and unique.

4.3 Analytical Example: The Allen-Cahn (Bistable) Equation

We can extend the argument above to the bistable case. For $\theta \in (0, 1)$, $\mu > 0$, $\nu > 0$, consider the discontinuous function

$$f(u) = \begin{cases} -\nu u & \text{for } \; 0 \leq u < \theta, \\ \mu(1-u) & \text{for } \; \theta < u \leq 1. \end{cases} \tag{4.6}$$

Lemma 4.3 *For f given by (4.6), there is a unique solution (c^*, v) of (4.2) with v decreasing and normalized with $v(0) = \theta$.*

Proof Again we may compute the unique solutions of the linear equations in $(-\infty, 0)$ and $(0, \infty)$. For $x > 0$, the equation is $v'' + cv' - \nu v = 0$; the characteristic polynomial $\lambda^2 + c\lambda - \nu = 0$ has a unique negative root that gives us

$$v(x) = \theta e^{-\lambda_r x}, \qquad \lambda_r = \frac{1}{2}\left[c + \sqrt{c^2 + 4\nu}\right].$$

The same occurs for $x < 0$, the equation is $v'' + cv' - \mu(1-v) = 0$, that is, $v = 1-w$ with $w'' + cw' - \mu w = 0$. This is a linear differential equation and the solutions are exponentials $e^{\lambda x}$ with $\lambda^2 + c\lambda - \mu = 0$. Therefore, there is a unique solution which is decaying to 0 at infinity and it is given by

$$v(x) = 1 - (1-\theta)e^{\lambda_l x}, \qquad \lambda_l = \frac{1}{2}\left[-c + \sqrt{c^2 + 4\mu}\right].$$

To match the derivatives at $x = 0$, we have to impose

$$\lambda_r(c)\theta = (1-\theta)\lambda_l(c).$$

Observe that $2\frac{d}{dc}\lambda_r(c) = 1 + \frac{c}{\sqrt{c^2+4\nu}} > 0$ and $2\frac{d}{dc}\lambda_l(c) = -1 + \frac{c}{\sqrt{c^2+4\mu}} < 0$ and that the limits at $\pm\infty$ of $\lambda_{r,l}$ are $\pm\infty$. This shows there is a unique c that makes the equality. $\square$

Again, the traveling speed c^* results from a combination of the solution behind and in front of the transition point $x = 0$ and we still have a pushed front.

Exercise Build a similar example with $u = 0$, $u = 1$ unstable and conclude there is no traveling wave connecting these states.

4.4 Analytical Example: The Fisher/KPP Equation

For $\theta \in (0, 1)$, $\mu > 0$, consider the continuous piecewise linear function

$$f(u) = \begin{cases} \mu(1-\theta)u & \text{for } 0 \le u \le \theta, \\ \mu\theta(1-u) & \text{for } \theta \le u \le 1. \end{cases} \tag{4.7}$$

Lemma 4.4 *For f given by (4.7), there is a minimal speed $c^* = 2\sqrt{\mu(1-\theta)}$; for all $c \ge c^*$ there is a unique solution (c, v) of (4.2) normalized by $v(0) = \theta$ and with v decreasing.*

The solution v *decays exponentially to* 0 *with the 'slowest possible' rate of decay of the corresponding equation (see below, for* $c = c^*$ *it is* $xe^{\lambda_- x}$ *not* $e^{\lambda_- x}$*).*

Therefore, the situation is very different from the case of Lemma 4.2 where there is a unique wave speed.

Proof For $x < 0$, we want $v > \theta$ and the equation is

$$-cv' - v'' = \mu\theta(1 - v).$$

Therefore, we find as in the proof of Lemma 4.2 that the unique solution that tends to 1 at $-\infty$ is given by

$$v = 1 - (1 - \theta)e^{\lambda_+ x}, \quad x \le 0, \qquad \lambda_+ = \frac{1}{2}\left[-c + \sqrt{c^2 + 4\mu\theta}\,\right].$$

For $x > 0$, the equation is written as $cv' + v'' + \mu(1 - \theta)v = 0$. The new feature is that both roots to the characteristic polynomial $\lambda^2 + c\lambda + \mu(1 - \theta)$ are negative. Thus, there is a one parameter family of solutions which decay to 0 at infinity

$$v = \theta e^{\mu_- x} + a(e^{\mu_+ x} - e^{\mu_- x}), \quad x \ge 0 \qquad \mu_\pm = \frac{1}{2}\left[-c \pm \sqrt{c^2 - 4\mu(1 - \theta)}\,\right] < 0.$$

Note that v is positive if, and only if, $a \ge 0$.

It remains to check that the derivatives match at $x = 0$, that is

$$-(1 - \theta)\lambda_+ = \theta a\mu_- + a(\mu_+ - \mu_-).$$

or, making explicit the various expressions, our result is reduced to checking that

$$-(1-\theta)\left[-c + \sqrt{c^2 + 4\mu\theta}\,\right] = -\theta\left[c + \sqrt{c^2 - 4\mu(1 - \theta)}\,\right] + 2a\sqrt{c^2 - 4\mu(1 - \theta)}\,,$$

$$c - (1 - \theta)\sqrt{c^2 + 4\mu\theta} + \theta\sqrt{c^2 - 4\mu(1 - \theta)} = 2a\sqrt{c^2 - 4\mu(1 - \theta)}\,.$$

For any $c > c^*$, the left hand side is a positive quantity (this is left as an exercise). Consequently, we can compute a unique $a > 0$ that satisfies this equality. This corresponds to a positive and decreasing function v.

For $c = c^*$ see the exercise below. □

Here we observe a different situation than before. The minimal traveling speed c^* is solely determined by the solution in front of the transition point $x = 0$ (in fact by the decay at $+\infty$). For that reason it is called a pulled front see J. Garnier et al. [18].

Exercise Consider the case $c = c^*$.

1. Show that for $x > 0$, v is given by $\theta e^{\mu - x} + \tilde{a} x e^{\mu - x}$ with $\tilde{a} > 0$.
2. Compute the compatibility relation for the derivatives.
3. Show that there is a unique solution (decaying or with values in $(0, 1)$).

Exercise For $0 < c < c^*$

1. Prove that there is no positive traveling wave.
2. Prove there may exist traveling waves but they change sign (oscillate) around $x = +\infty$, $v \approx 0$.

Exercise For $\theta \in (0, 1)$, $\mu > 0$, $\nu > 0$ we define the discontinuous piecewise linear function

$$f(u) = \begin{cases} \nu\, u & \text{for } 0 \le u < \theta, \\ \mu\, (1 - u) & \text{for } \theta < u \le 1. \end{cases} \tag{4.8}$$

We consider the traveling wave problem, that is, to find for which c there is a decreasing solution v to

$$\begin{cases} -v''(x) - cv'(x) = f\big(v(x)\big), \qquad x \in \mathbb{R}, \\ \\ v(-\infty) = 1, \qquad v(+\infty) = 0, \qquad v(0) = \theta. \end{cases} \tag{4.9}$$

We always assume that $c > 2\sqrt{\nu}$.

1. Give the expression of v for $x < 0$.
2. Give the one parameter family of decreasing solutions for $x > 0$ and indicate the condition for the parameter.
3. Give the matching condition on v' at $x = 0$.
4. Characterize the minimal speed c^* which is defined such that for $c > c^*$ one can find a traveling wave, for $c < c^*$ there is no traveling wave.

Hint. The relation which gives the free parameter is

$$F(c) := c - (1 - \theta)\sqrt{c^2 + 4\mu} \; + \theta\sqrt{c^2 - 4\nu} \; = 2a\sqrt{c^2 - 4\nu} > 0.$$

The function F is increasing in c. Therefore, for ν sufficiently large, the minimal speed is defined by $c^* = 2\sqrt{\nu}$; this is as long as $F(2\sqrt{\nu}) > 0$, that is, $\nu > \mu\, \frac{(1-\theta)^2}{\theta(2-\theta)}$. For ν smaller, then $F(2\sqrt{\nu}) < 0$ and c^* is defined by $F(c^*) = 0$.

The interest here is to show that $c^* > 2\sqrt{\nu}$ when ν is small, and thus there is an interesting question to understand the general rule for this minimal speed.

4.5 Analytical Solutions: Non-local Fisher/KPP Equation (Problem)

We give $\theta \in (0, 1)$ and define $K * u(x) = \int_{\mathbb{R}} K(x-y)u(y)dy$ with

$$K(z) = \mathbf{1}_{\{z>0\}} e^{-z}.$$

We look for a bounded traveling wave solution $\big(c > 0, u(x)\big)$ to

$$\begin{aligned} &-u''(x) - cu'(x) = \begin{cases} 0 & \text{for } 0 \le u < \theta, \\ 1 - K * u & \text{for } \theta < u. \end{cases}, \qquad x \in \mathbb{R}, \\ &u(-\infty) = 1, \qquad u(+\infty) = 0, \qquad u(0) = \theta. \end{aligned} \tag{4.10}$$

For $x < 0$, we look for a complex solution $u(x) = 1 - (1-\theta)e^{(\lambda+i\mu)x}$ with $\lambda > 0$.

1. Show that $\mathbf{u}(x)$ is solution if, and only if,

$$c(\lambda + i\mu) + (\lambda + i\mu)^2 = \frac{1}{\lambda + i\mu + 1}.$$

2. Show that the only possibility is $\mu = 0$.
3. For $x > 0$, give the solution $u(x) \le \theta$.
4. Write the matching condition between $u(x)$, $x > 0$ and $u(x)$ at $x = 0$.
5. What can we conclude on the problem (4.10)? Is this result usual?

Solution

1. Because $\lambda > 0$, we have $|e^{(\lambda+i\mu)x}| < 1$ and $Re u(x) > \theta$ so that we can use the equation

$$-u''(x) - cu'(x) = 1 - K * u, \qquad x < 0.$$

Also the support of K ensures that $x - y > 0$ and thus, the above problem is self-contained (it does not use $u(x)$ for $x > 0$). It remains to note that $K * 1 = 1$ (K is a probability kernel) and

$$K * \mathbf{u}(x) = 1 - (1-\theta)e^{(\lambda+i\mu)x} \int K(x-y)e^{(\lambda+i\mu)(y-x)}dy = 1 - \frac{1-\theta}{\lambda + i\mu} e^{(\lambda+i\mu)x}$$

and the result follows immediately.

2. We write the relation as

$$c(\lambda + i\mu) + (\lambda + i\mu)^2 = \frac{\lambda - i\mu + 1}{|\lambda + 1|^2 + |\mu|^2}.$$

The imaginary part of which gives

$$\mu[c + 2\lambda] = -\frac{\mu}{|\lambda + 1|^2 + |\mu|^2}.$$

Apart from $\mu = 0$, the solution is $c + 2\lambda = -\frac{1}{|\lambda+1|^2+|\mu|^2} < 0$ but both c and λ are positive and this is impossible.

3. $u = \theta e^{-cx} < \theta$ is the only solution of $-u'' - cu' = 0$ with $u(0) = \theta$ and $u(\infty) = 0$.
4. We have to write that $u'(0^-) = u'(0^+)$. That is, $c\theta = (1 - \theta)\lambda$.
5. The problem is reduced to find $c > 0$ and $\lambda > 0$ such that the above relations hold: $c\lambda + \lambda^2 = \frac{1}{\lambda+1}$, $c = \alpha\lambda$ with $\alpha = \frac{1-\theta}{\theta}$. That is

$$(\alpha + 1)\lambda^2 = \frac{1}{\lambda + 1}.$$

Because the right hand side is increasing from 0 to $+\infty$ and the left hand side is decreasing there is a single solution λ and thus a single c.

Therefore, we have built a unique decreasing traveling wave. This is the usual result.

4.6 The Monostable (Fisher/KPP) Equation with Ignition Temperature

The Fisher/KPP equation with ignition temperature appears in the theory of combustion when a minimum 'temperature' $0 < \theta < 1$ is required to burn the gas. It gives the model

$$\frac{\partial}{\partial t}u - \frac{\partial^2}{\partial x^2}u = f(u), \qquad t \geq 0,\ x \in \mathbb{R}. \tag{4.11}$$

with a smooth reaction term given by

$$f_\theta(u) = \begin{cases} 0 & \text{for } 0 \leq u \leq \theta, \\ > 0 & \text{for } \theta < u < 1, \end{cases} \qquad f(1) = 0. \tag{4.12}$$

The traveling wave problem is still to find c and v such that

$$\begin{cases} -v''(x) - cv'(x) = f\big(v(x)\big), & x \in \mathbb{R}, \\ v(-\infty) = 1, \qquad v(+\infty) = 0. \end{cases} \tag{4.13}$$

We are going to prove the

Theorem 4.5 *For the Fisher/KPP equation with ignition temperature, i.e.,* (4.11) *when $f(\cdot)$ satisfies* (4.12)*, there is a unique decreasing traveling wave solution (c^*, v) normalized with $v(0) = \frac{1}{2}$ and it holds that $c^* > 0$.*

Much more is known about this problem, see [31]. For instance, we give below explicit bounds on c^*.

Proof The easiest proof relies on the *phase space* method for O.D.Es, which we follow here. It is however limited to simple problems and more advanced PDE methods can be found in [31].

We decompose the proof into three steps: (i) we reduce the problem to a simpler O.D.E. (ii) we prove the monotonicity in c (iii) we prove existence.

First Step. Reduction to an ODE We reduce the traveling wave problem to an O.D.E. problem. We fix c and set $w = -v'$ (so that $w > 0$ because we look for decreasing v). Then, Eq. (4.13) becomes a system of differential equations

$$\begin{cases} v' = -w, \\ w' = -c\, w + f(v), \\ v(-\infty) = 1, \; w(-\infty) = 0, \qquad v(+\infty) = 0, \; w(+\infty) = 0. \end{cases} \tag{4.14}$$

It can be further simplified because by monotonicity, we can invert $v(x)$ as a function $X(v)$, $0 \le v \le 1$ and define a function $\tilde{w}(v) = w(X(v))$. In place of (4.14), we have to find a solution of

$$\begin{cases} \dfrac{d\tilde{w}(v)}{dv} = \dfrac{dw}{dx}\,\Big(\dfrac{dv}{dx}\Big)^{-1} = c - \dfrac{f(v)}{\tilde{w}}, \quad 0 \le v \le 1, \\ \tilde{w}(0) = \tilde{w}(1) = 0, \qquad \tilde{w} \ge 0. \end{cases}$$

Therefore, we arrive at the question to know if the solution of the Cauchy problem

$$\begin{cases} \dfrac{d\tilde{w}_c(v)}{dv} = c - \dfrac{f(v)}{\tilde{w}_c(v)}, \qquad 0 \le v \le 1, \\ \tilde{w}_c(0) = 0, \end{cases} \tag{4.15}$$

can also achieve, for a special value of c, the conditions

$$\tilde{w}_c(1) = 0, \quad \tilde{w}_c(v) \ge 0, \text{ for } 0 \le v \le 1. \tag{4.16}$$

Notice that there is a possible singularity at $v = 0$ because the numerator and denominator vanish in the right hand side of (4.15). But for $0 \le v \le \theta, f(v) \equiv 0$ and the solution is simply

$$\tilde{w}_c(v) = c\ v, \qquad 0 \le v \le \theta.$$

Then it can be continued smoothly as a simple (nonsingular) O.D.E. until either we reach $v = 1$, or $\tilde{w}_c$ vanishes and the problem is not defined any longer. Numerics indicate that, depending on c, either we have

- $\tilde{w}_c(v) > 0$ for $0 \le v \le 1$ (call it Type I), then we set $v_c = 1$, or
- $\tilde{w}_c(v_c) = 0$ for some $0 < v_c < 1$ (call it Type II), then the equation tells us that $\tilde{w}'_c(v_c) = -\infty$.

In both cases these are not solutions because they cannot fulfill (4.16). In the limiting case $v_{c^*} = 1$ there is a solution. These possible behaviors are depicted in Fig. 4.3.

Second Step. Monotonicity in *c* We now prove that this last case can only occur for a single v_c based on the

Lemma 4.6 *The mapping $c \mapsto \tilde{w}_c(v)$ is increasing for those values of v where it is defined, i.e., for $0 < v < v_c$. Moreover for $c' > c$ we have $v_{c'} > v_c$ (and $v_{c'} = v_c$ if $v_c = 1$) and*

$$\tilde{w}_{c'}(v) \ge \tilde{w}_c(v) + (c' - c)\ v, \qquad 0 \le v \le v_c. \tag{4.17}$$

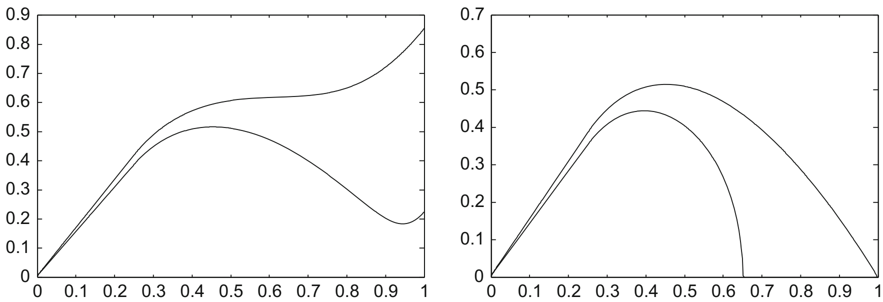

Fig. 4.3 Traveling wave solutions to the Fisher/KPP equation with temperature ignition (4.13) with threshold $\theta = 0.25$ plotted in the phase space variables (4.15). We have plotted four different values of c. The x-axis represents v and the y-axis represents the function $\tilde{w}(v)$. *Left*: two cases where the solution of (4.15) does not vanish (large c), these are called Type I. *Right*: the limiting case $c = c^*$ and a smaller value of c, these are called Type II. Note that the w scale is larger on the *left* than on the *right*

Proof Set $z_c(v) = \frac{d\tilde{w}(v)}{dc}$. It satisfies,

$$\frac{dz_c(v)}{dv} = 1 + \frac{f(v)}{\tilde{w}(v)^2}\, z_c(v), \qquad z_c(0) = 0.$$

From this equation we deduce that z_c cannot vanish and thus $z_c(v) \geq v$ as long as it is defined, i.e., that $\tilde{w}_c(v)$ does not vanish for $0 \leq v < v_c$. The conclusions follow.

After integration in c we find the desired inequality on $\tilde{w}$, which holds up to $v = v_c$ by continuity. □

Consequently, $\tilde{w}_c(1)$ is an increasing function of c. Therefore, there can indeed be at most one value of c satisfying the condition $\tilde{w}_c(1) = 0$.

Third Step. Bounds on *c* We introduce the two positive real numbers defined (uniquely) by

$$\underline{c}^2 = \int_0^1 \frac{f(v)}{v}\, dv, \qquad \bar{c}^2 = 4 \max_{0 \leq v \leq 1} \frac{f(v)}{v}.$$

Notice that $\underline{c} < \bar{c}$. In fact we are going to prove that

Lemma 4.7 *For $c > \bar{c}$, the solution is of Type I. For $c \leq \underline{c}$, the solution is of Type II and*

$$\underline{c} < c^* \leq \bar{c}. \tag{4.18}$$

Proof **Estimate from Above** We first show that for $c > \bar{c}$, the solution is of Type I. We consider the largest interval $[0, v_0] \subset [0, 1]$ on which $\tilde{w}_c(v) \geq \frac{c}{2} v$. Because $\tilde{w}_c(v) = c\ v$ in $[0, \theta]$ clearly $v_0 > \theta$. If $v_0 < 1$ (otherwise we are done), then $\tilde{w}'_c(v_0) \leq \frac{c}{2}$. Then, for $\theta \leq v \leq v_0$, we have

$$\frac{c}{2} \geq \frac{d\tilde{w}_c(v_0)}{dv} \geq c - 2\frac{f(v_0)}{c\ v_0} \geq c - \frac{\bar{c}^2}{2c},$$

which is a contradiction. This means that $v_0 = 1$ and the situation is of Type I.

Estimate from Below We show that for $c \leq \underline{c}$ the solution is of Type II. We remark that $\tilde{w}_c(v) \leq cv$ as long as it is defined (because $\frac{f(v)}{\tilde{w}(v)} \geq 0$) and thus

$$\frac{d\tilde{w}_c(v)}{dv} = c - \frac{f(v)}{\tilde{w}_c(v)} \leq c - \frac{f(v)}{cv}.$$

Because the inequality is strict for $v > \theta$, we obtain

$$\tilde{w}_c(v) \leq c\ v - \int_0^v \frac{f(s)}{cs} ds.$$

This implies that, if the solution did not vanish before $v = 1$, we would have $0 \leq \tilde{w}_c(1) < c - \int_0^1 \frac{f(s)}{cs} ds$. This implies that $\underline{c} < c$. This proves that the solution is of Type II for $c \leq \underline{c}$. □

Fourth step. Conclusion We can conclude the proof by a continuity argument on v_c in the region of Type II. By the monotonicity argument of step (ii) and because of (4.17) as long as $v_c < 1$, the point v_c increases continuously with controlled uniform growth (see exercise below). Therefore, $\max_c v_c = 1$, where the *max* is taken on the c of Type II, and it is achieved for $c = c^*$, in other words $v_{c^*}(1) = 0$. When $c > c^*$, the solution is of Type I again by the monotonicity argument (we know from Lemma 4.6 that $\tilde{w}_c(1)$ decreases uniformly with c). □

Exercise Find a lower bound on $\frac{d}{dc} v_c$. Prove it is positive as long as $v_c < 1$ and that it is uniformly positive for $v_c \approx 1$.

Hint. $c \int_0^{v_c} \tilde{w}_c(v)dv = \int_0^{v_c} f(v)dv$. Also use the information in the proof to conclude that

$f(v_c)\frac{dv_c}{dc} = \int_0^{v_c} \tilde{w}_c(v)dv + c\int_0^{v_c} z_c(v)dv \geq \frac{c}{2}\theta^2 + \frac{c}{2}(v_c)^2.$

Exercise For $\varepsilon > 0$, study the (regularized) Cauchy problem

$$\begin{cases} \dfrac{dw}{dv} = c - \dfrac{f(v)}{\sqrt{\varepsilon^2 + w(v)^2}}, \qquad 0 \leq v \leq 1, \\ w(0) = 0. \end{cases} \tag{4.19}$$

(1) Show that one cannot achieve $w(1) = 0$ with $w(v) \geq 0$ for $0 \leq v \leq 1$ whatever are c or ε.
(2) Show that, for all values of v, the mapping $c \mapsto w_{c,\varepsilon}(v)$ is increasing and the mapping $\varepsilon \mapsto w_{c,\varepsilon}(v)$ is non-decreasing.
(3) For ε fixed, show that one can find a unique c^ε that achieves $w(v_\varepsilon) = 0$, $w(v) \geq 0$ in a maximal interval $0 \leq v \leq v_\varepsilon$. What is the value $w'_{c^\varepsilon,\varepsilon}(v_\varepsilon)$?
(4) Draw the solutions for several values of c.
(5) Prove that $v_\varepsilon \to 1$, $c^\varepsilon \to c^*$ as $\varepsilon \to 0$.

Solution

(1) Indeed, this implies $w'(1) \geq 1$ but the equation implies that $w'(1) = c > 0$.
(2) Same proof as above.
(3) As in the above proof, for $c^2 > \|f\|_\infty/\theta$, we have $w'_c(v) > 0$ and for $c < c_*$ we have $w_c(1) < 0$ with c_* the unique fixed point of $c_* = \int_0^1 f(v)/\sqrt{\varepsilon^2 + c_*^2 v^2} dv$. So, by monotonicity, there is a larger $c = c^\varepsilon$ such that w vanishes at some point, $w(v_\varepsilon) = 0$ and $w(v) \geq 0$. Therefore, we have $w'(v_\varepsilon) = 0$, which implies $\varepsilon c^\varepsilon = f(v_\varepsilon)$.
(4) As ε decreases to 0, one can check (still by monotonicity) that c^ε increases to a limit $c_f > c_*$. On the other hand, from the previous question, $f(v_\varepsilon) \to 0$. One checks that v_ε remains far from $[0, \theta]$ and thus, from the assumption on f,

we have $v_\varepsilon \to 1$. In the limit we obtain a solution of (4.15) which vanishes at $v = 1$.

4.7 Allen-Cahn (Bistable) Equation

Uniquely defined traveling wave solutions may exist for other nonlinearities. In this section we study the *bistable* nonlinearity related to the O.D.E.

$$\frac{d}{dt}u(t) = u(t)\,\big(1 - u(t)\big)\,\big(u(t) - \theta\big),$$

for some parameter

$$0 < \theta < 1. \tag{4.20}$$

Here the function $f(\cdot)$ has three steady states, $u \equiv 0$ and $u \equiv 1$ are stable, $u \equiv \theta$ is unstable. Any solution will converge either to 0, for $u^0 < \theta$ or to 1 for $u^0 > \theta$. Also the region $0 \leq u^0 \leq 1$ is invariant with time.

Compared to the Fisher/KPP equation, the bistable (Allen-Cahn) equation uses an improvement of the logistic growth term $u(1-u)$; this supposes that too low population densities $u(t)$, less than θ, lead to extinction by lack of encounters between individuals. This is called the Allee effect [1]. It however takes its name from the theory of phase transitions [2].

Next, we include motion of individuals and we obtain the Allen-Cahn equation

$$\frac{\partial}{\partial t}u(t,x) - \Delta u(t,x) = u(t,x)\big(1 - u(t,x)\big)\big(u(t,x) - \theta\big). \tag{4.21}$$

We look for traveling wave solutions $u(x,t) = v(x - ct)$, with $v(\cdot)$ solution of

$$\begin{cases} -cv'(x) - v''(x) = v(x)\big(1 - v(x)\big)\big(v(x) - \theta\big), \\ v(-\infty) = 1, \qquad v(+\infty) = 0, \qquad v(0) = \frac{1}{2}. \end{cases} \tag{4.22}$$

We have again imposed the condition $v(0) = \frac{1}{2}$ to avoid the translational invariance.

The following result is similar to the case of the Fisher/KPP equation with ignition temperature:

Theorem 4.8 *There exists a unique decreasing solution* (c^*, v) *of* (4.22) *and*

$$c^* > 0 \quad \textit{for}\ \ 0 < \theta < \frac{1}{2}, \qquad c^* = 0 \quad \textit{for}\ \ \theta = \frac{1}{2}, \qquad c^* < 0 \quad \textit{for}\ \ \frac{1}{2} < \theta < 1.$$

The sign follows from the general principle in Sect. 4.1.

Theorem 4.8 is a consequence of the explicit solution that we leave as an exercise:

Exercise Set $u(x) = \frac{e^{-x/\sqrt{2}}}{1+e^{-x/\sqrt{2}}}$.

1. Check that the corresponding traveling wave connects the state $u(-\infty) = 1$ to $u(\infty) = 0$.
2. Check that u satisfies Eq. (4.22) and write the relation between θ and c^*.

Solution $c^* = \sqrt{2}(\frac{1}{2} - \theta)$.

However, a general proof is available which does not use the specific form of the bistable nonlinearity but only the property that there is a unique root θ, $0 < \theta < 1$ such that

$$\begin{cases} f(0) = 0,\, f'(0) < 0, \qquad f(\theta) = 0, \qquad f(1) = 0,\, f'(1) < 0, \\ f(u) < 0 \quad \text{for } 0 < u < \theta, \qquad\qquad f(u) > 0 \quad \text{for } \theta < u < 1. \end{cases} \tag{4.23}$$

Following again the general principle in Sect. 4.1, the speed of the wave then depends upon the sign of $W(1)$ with

$$W(u) = \int_0^u f(v)dv.$$

Theorem 4.9 *With the assumption* (4.23)*, there exists a unique traveling wave* (c^*, v) *of* (4.22) *with* v *decreasing and*

$$c^* > 0 \mathit{for} \;\; W(1) < 0, \qquad c^* = 0 \quad \mathit{for} \;\; W(1) = 0, \qquad c^* = 0 \quad \mathit{for} \;\; W(1) > 0.$$

Proof As in Sect. 4.6, we consider (4.22) as an O.D.E. that we solve as a system of first order equations

$$\begin{cases} v'(x) = -w(x), \\ w'(x) = -c\, w(x) + f\big(v(x)\big), \\ v(-\infty) = 1,\; w(-\infty) = 0, \qquad v(+\infty) = 0,\; w(+\infty) = 0. \end{cases}$$

And because we look for v decreasing, we can invert $v(x)$ as a function $X(v)$, $0 \le v \le 1$ and define a function $\tilde{w}(v) = w(X(v))$. Following the derivation of (4.15) in the case of the Fisher/KPP equation with ignition temperature, we arrive here to

$$\begin{cases} \dfrac{d\tilde{w}(v)}{dv} = c - \dfrac{f(v)}{\tilde{w}(v)}, \qquad 0 \le v \le 1, \\ \tilde{w}(0) = \tilde{w}(1) = 0, \qquad\qquad \tilde{w} \ge 0. \end{cases} \tag{4.24}$$

Then, we consider the case $W(1) > 0$ only (otherwise the argument is the same except we have to argue departing from $v = 1$). We argue in several steps.

(i) First, the singularity of the right hand side at $v = 0$ can be handled with L'hospital rule and computing from (4.24)

$$\tilde{w}'(0) - \frac{f'(0)}{\tilde{w}'(0)} = c \iff \tilde{w}'(0) = S(c),$$

and the function $c \mapsto S(c) = \frac{1}{2}\left(c + \sqrt{c^2 + 4|f'(0)|}\right)$ is increasing.

This allows (using a version of the Cauchy-Lipschitz theorem with singularities at the origin) to define a unique solution of

$$\begin{cases} \dfrac{d\tilde{w}_c(v)}{dv} = c - \dfrac{f(v)}{\tilde{w}_c(v)}, \\ \tilde{w}(0) = 0, \qquad \tilde{w}_c'(0) = S(c). \end{cases} \tag{4.25}$$

Because $f(v) \le 0$ in $[0, \theta]$, we have $\frac{d\tilde{w}_c(v)}{dv} \ge c$ and thus

$$\tilde{w}_c(v) \ge cv \quad \text{on } [0, \theta].$$

Therefore, $\tilde{w}_c$ is either defined and positive for all $0 \le v \le 1$, then we set $v_c = 1$ and call it Type I. Or it is defined in an interval $[0, v_c]$ with $\tilde{w}_c(v_c) = 0$ and

$$v_c > \theta, \tag{4.26}$$

when the system reaches another singularity where $\tilde{w}_c'(v_c) = -\infty$, and then we call it Type II.

(ii) The property holds

$$c \mapsto \tilde{w}_c(v) \quad \text{is } C^1 \text{ and increasing for } 0 < v \le v_c.$$

Indeed, following the Fisher/KPP case, we set $z_c(v) = \tilde{w}_c(v)'$ and we have

$$\begin{cases} \dfrac{dz_c(v)}{dv} = 1 + z_c(v)\dfrac{f(v)}{\tilde{w}_c(v)^2}, \\ z_c(0) = 0, \qquad z_c'(0) = S'(c) > \frac{1}{2}. \end{cases}$$

Near $v = 0$, the solution of this equation is positive. It remains positive for all $v > 0$ because if $z_c(v)$ becomes too small the equation tells us that its derivative is positive.

(iii) It is easy to conclude that, for c sufficiently large, $\tilde{w}_c(v)$ remains increasing in $[0, 1]$. In other words, for c large enough the solution is of type I.

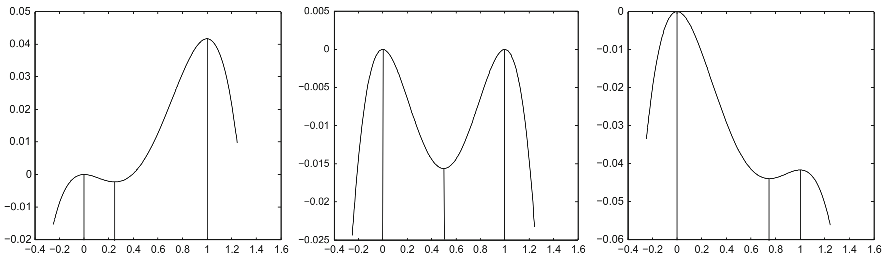

Fig. 4.4 The function $W(u) = \int_0^u v(1-v)(v-\theta)dv$ for different values of θ. *Left*: $\theta = 0.25$ and W is negative for $(0, \beta)$ for some $\beta > \theta$ and positive in $]\beta, 1]$. *Center*: $\theta = 0.5$ and $W(u)$ is nonpositive and vanishes at $u = 0$ and $u = 1$. *Right*: $\theta = 0.75$ and W is negative in $(\beta, 1)$ for some $\beta < \theta$

We claim that the solution for $c \approx 0$ is of type II. Indeed, we can compute another relation because the equation reads

$$\frac{1}{2}\frac{d\,\tilde{w}_c(v)^2}{dv} = c\tilde{w}_c - f(v) = c\tilde{w}_c - W'(v),$$

with $W(v) = \int_0^v f(z)dz$ depicted in Fig. 4.4. We arrive at

$$\frac{1}{2}\tilde{w}_c(v)^2 = c\int_0^v \tilde{w}_c(z)dz - W(v). \tag{4.27}$$

For $c = 0$ this gives

$$\tilde{w}_0(v)^2 = -2W(v).$$

Because $W(v) \le 0$ in $[0,1]$ only when $\theta = 1/2$, this shows that $c = 0$ gives the *standing wave* (traveling wave with speed 0). For $\theta < 1/2$, W vanishes at a point that we denote by β

$$W(\beta) = 0, \qquad 1/2 < \beta < 1.$$

In other words $c = 0$, and by continuity $c \approx 0$, give a solution of Type II.

(iv) As c increases from $c = 0$, v_c also increases thanks to the item (ii) and we can write from (4.27)

$$0 = c\int_0^{v_c} \tilde{w}_c(z)dz - W(v_c), \qquad \tilde{w}_c(v_c) = 0.$$

Differentiating in c, we obtain

$$0 = \int_0^{v_c} \tilde{w}_c(z)dz + c\tilde{w}_c(v_c)\frac{dv_c}{dc} - W'(v_c)\frac{dv_c}{dc} = \int_0^{v_c} \tilde{w}_c(z)dz - W'(v_c)\frac{dv_c}{dc},$$

or also, recalling (4.26),

$$\frac{dv_c}{dc} = \frac{\int_0^{v_c} \tilde{w}_c(z)dz}{f(v_c)} > 0.$$

So that we can define again c^* as the maximum of the c corresponding to type II. It has to satisfy $\tilde{w}_{c^*}(v_{c^*}) = 0$. By strong monotonicity, or by (4.27), it is also the minimum of c giving solutions of type I. □

4.8 The Fisher/KPP Equation

We can now come back to the more basic Fisher/KPP equation

$$\nu v''(x) + cv'(x) + rv(x)\big(1 - v(x)\big) = 0, \qquad x \in \mathbb{R}, \tag{4.28}$$

$$v(-\infty) = 1, \qquad v(+\infty) = 0, \qquad v(0) = 1/2, \tag{4.29}$$

and, again, the last condition is to fix the translational invariance.

The situation here is very different from the case with ignition temperature and from the Allen-Cahn equation. A famous result [3] is the

Theorem 4.10 *For any $c \geq c^* := 2\sqrt{\nu r}$, there is a unique (traveling wave) solution v, $0 \leq v(x) \leq 1$, of (4.28)–(4.29). It is monotonically decreasing.*

The quantity c^* is called the *minimal propagation speed*. This speed c^* corresponds, in several senses, to the most stable traveling wave; we mention one example later based on perturbation of the nonlinear term by including an ignition temperature θ and letting θ vanish. It is also the type of wave that appears as the long term limit of the evolution equation with compactly supported initial data. See [31].

The condition $c \geq c^*$ can be derived from studying the 'tail' of $v(x)$ for x close to $+\infty$. Because $v = 0$ is unstable, we can look for exponential decay as $x \approx \infty$, namely

$$v(x) \approx e^{-\lambda x}, \quad x \gg 1, \qquad \lambda > 0.$$

Inserting this in (4.28), we find

$$\nu\, \lambda^2 - c\, \lambda + r = 0, \quad \lambda = \frac{c \pm \sqrt{c^2 - 4\nu r}}{2\nu}. \tag{4.30}$$

Because no oscillation can occur around $v = 0$ (due to the condition $v > 0$) we should have $c^2 \geq c^{*2} = 4\nu r$. And $c > 0$ is required to have $\lambda > 0$, hence we should have $c \geq c^*$.

The Fisher/KPP equation can be extended to a more general right hand side

$$\frac{\partial}{\partial t}u - \nu \frac{\partial^2}{\partial x^2}u = f(u), \qquad t \geq 0,\ x \in \mathbb{R}, \tag{4.31}$$

with $f : \mathbb{R} \to \mathbb{R}$ a smooth mapping satisfying

$$f(0) = f(1) = 0, \qquad f(u) > 0 \text{ for } 0 < u < 1.$$

When f is concave in $[0, 1]$ (this is the case of the Fisher/KPP term $u(1-u)$), the linearization method explained above and Theorem 4.10, remains true with the slight modification that the minimal propagation speed is now

$$c^* = 2\sqrt{f'(0)\nu}.$$

We do not give a complete proof and refer the interested reader to [14, 31]. We only indicate the difficulties and two ways to solve them.

Proof of Theorem 4.10 (Phase Space) If we try the *phase space* method as before, we set $w = -v'$. Then, the system (4.28) becomes

$$\begin{cases} v' = -w, \\ w' = -\frac{c}{\nu}\, w + \frac{r}{\nu}\, v(1-v), \\ v(-\infty) = 1,\ w(-\infty) = 0, \qquad v(+\infty) = 0,\ w(+\infty) = 0. \end{cases} \tag{4.32}$$

This can be further simplified, because by monotonicity we can still invert $v(x)$ as a function $X(v)$ and define a function $\tilde{w}(v) = w(X(v))$. In place of (4.32), we have to find a solution for

$$\begin{cases} \dfrac{d\tilde{w}(v)}{dv} = \dfrac{dw}{dx}\,\Big(\dfrac{dv}{dx}\Big)^{-1} = \dfrac{c}{\nu} - \dfrac{r}{\nu}\,\dfrac{v(1-v)}{\tilde{w}}, \quad 0 \leq v \leq 1, \\ \tilde{w}(0) = \tilde{w}(1) = 0, \qquad \tilde{w} \geq 0. \end{cases} \tag{4.33}$$

This differential equation still has a singularity at $v = 0$ and $v = 1$ but it is worse than we encountered before. If we try to guess what is the slope $\tilde{w}'(0)$, we find

$$\tilde{w}'(0) = \frac{c}{\nu} - \frac{r}{\nu}\,\frac{1}{\tilde{w}'(0)}, \qquad \tilde{w}'(0) = \frac{1}{2\nu}[c \pm \sqrt{c^2 - 4\nu r}].$$

This confirms that we can only begin the trajectory when $c \geq c^*$, but does not tell us which branch to use.

Instead, we can argue by perturbation and consider a family $\theta \to 0$ in the model with ignition temperature (4.12). We denote the corresponding solution by $(c^*(\theta), \tilde{w}^\theta(v))$. For a well-tuned f_θ in (4.12) we have

$$f_\theta(u) \to ru(1-u) \quad \text{as } \theta \to 0, \qquad \text{in } C([0,1]),$$

and the lower and upper bounds $(\underline{c}(\theta), \bar{c}(\theta))$ in Lemma 4.7 are uniformly bounded in θ. Therefore, we can extract a subsequence

$$\theta_n \to 0, \qquad c^*(\theta_n) \to c^{**}, \qquad 0 < c^{**} < \infty.$$

On the other hand from (4.15), we know that $\tilde{w}^{\theta\prime}(v) \le c^*(\theta)$ and thus

$$0 \le \tilde{w}^\theta(v) \le c^*(\theta)v.$$

Writing

$$-\max_{0 \le v \le 1} f^\theta(v) \le \frac{d}{dv}\frac{\tilde{w}^\theta(v)^2}{2} = c^*(\theta)\tilde{w}^\theta(v) - f^\theta(v) \le c^*(\theta)^2 v,$$

we conclude by the Ascoli theorem that, after further extraction, $\tilde{w}^\theta(v)^2$ converges uniformly. Therefore, for the uniform convergence, we have

$$\tilde{w}^{\theta_n}(v) \underset{n\to\infty}{\longrightarrow} \tilde{w}^{**}(v), \qquad 0 \le \tilde{w}^{**}(v) \le c^{**}\, v.$$

Therefore, from the equation above, $\frac{d}{dv}\frac{\tilde{w}^{\theta_n}(v)^2}{2}$ converges uniformly and we can write

$$\frac{d}{dv}\frac{\tilde{w}^{**}(v)^2}{2} = c^{**}\tilde{w}^{**}(v) - f(v).$$

We deduce that $\tilde{w}^{**}(v)$ remains uniformly positive in $(0,1)$ and, from (4.15), that $\frac{d}{dv}\tilde{w}^{\theta_n}(v)$ also converges locally uniformly to a solution of (4.33).

It is possible to prove that this solution is the traveling wave with minimal speed but we shall not do it here. □

Proof of Theorem 4.10 (Physical Space) We consider again the solution $\big(c^*(\theta), v^\theta(x)\big)$ to the model with ignition temperature (4.12). We prove uniform estimates in θ, showing that we can extract subsequences which converge. We do that in several steps. Here we do not indicate the dependency upon θ.

1st step. Uniform upper bound on $c^*(\theta) < c^* = 2$. This also uses the additional assumption $f^\theta(v) < f(v) = v(1-v)$ in $(0,1)$. We argue by contradiction and assume $c := c^*(\theta) \ge c^*$. We consider

$$0 < \lambda = \frac{c - \sqrt{c^2-4}}{2} < c, \qquad \lambda^2 - c\lambda + 1 = 0.$$

For A large enough we have $Ae^{-\lambda x} > v^\theta(x)$, because of the compared behavior at infinity, $v(-\infty) = 1$ and $v(x) \approx e^{-cx}$ at $+\infty$. Take the largest A where the two functions touch, that is

$$A_0 e^{-\lambda x_0} = v^\theta(x_0) \qquad Ae^{-\lambda x} > v^\theta(x),\ \forall x \neq x_0.$$

Then $v'(x_0) = \lambda A_0 e^{-\lambda x_0}$, $v''(x_0) \le \lambda^2 A_0 e^{-\lambda x_0}$, and thus, from Eq. (4.12)

$$0 = v''(x_0)+v'(x_0)+f^\theta(v(x_0)) < \lambda^2 - c\lambda + \frac{v^\theta(x_0)\big(1-v^\theta(x_0)\big)}{v^\theta(x_0)} \le \lambda^2 - c\lambda + 1 = 0,$$

a contradiction. This proves the inequality.

2nd step. Lower bound on $c^*(\theta)$. We derive it from two equalities. The first is obtained by integrating (4.13) from x_- to x_+

$$c\big(v(x_+) - v(x_-)\big) + \big(v'(x_+) - v'(x_-)\big) + \int_{x_-}^{x^+} f^\theta\big(v(x)\big)dx = 0,$$

and thus, passing to the limits $x_- \to -\infty$, $x_+ \to \infty$, we find, thanks to the conditions at infinity

$$c^*(\theta) = \int_{-\infty}^{\infty} f^\theta\big(v^\theta(x)\big)dx. \tag{4.34}$$

We can also multiply by v in Eq. (4.13) and integrate. We find

$$\frac{c}{2}\big(v^2(x_+) - v^2(x_-)\big) + \big(vv'(x_+) - vv'(x_-)\big)$$
$$-\int_{x_-}^{x^+} \big(v'(x)\big)^2 dx + \int_{x_-}^{x^+} v(x) f^\theta\big(v(x)\big)dx = 0,$$

and in the limit

$$\frac{c^*(\theta)}{2} = \int_{-\infty}^{\infty} v^\theta(x) f^\theta\big(v^\theta(x)\big)dx - \int_{-\infty}^{\infty} \big(v^{\theta\prime}(x)\big)^2 dx. \tag{4.35}$$

Subtracting (4.35) to (4.34), we obtain

$$\frac{c^*(\theta)}{2} = \int_{-\infty}^{\infty} \big(1 - v^\theta(x)\big) f^\theta\big(v^\theta(x)\big)dx + \int_{-\infty}^{\infty} \big(v^{\theta\prime}(x)\big)^2 dx > 0 \qquad \text{(uniformly in } \theta). \tag{4.36}$$

3rd step. Uniform bound on v'. We multiply (4.13) by v' and obtain

$$c\,(v')^2 + \frac{1}{2}\big((v')^2\big)' + F^\theta\big(v(x)\big)' = 0,$$

with, for $0 \le v \le 1$,

$$F^\theta(v) = \int_0^v f^\theta(u)du \qquad \text{(a bounded increasing function).}$$

Integrating this equation as before and passing to the limits, we find

$$c^*(\theta)\int_{-\infty}^{\infty}\big(v^{\theta\prime}(x)\big)^2 dx = -\int_{-\infty}^{\infty} F^\theta\big(v^\theta(x)\big)' dx = F^\theta(1). \tag{4.37}$$

And integrating between y and ∞, we find

$$\frac{1}{2}\big(v^{\theta\prime}(y)\big)^2 = c^*(\theta)\int_y^{\infty}\big(v^{\theta\prime}(x)\big)^2 dx - F^\theta(y) \le F^\theta(1) - F^\theta(y). \tag{4.38}$$

4th step. Limit as $\theta \to 0$. These bounds combined with Eq. (4.13) prove that v'' is uniformly bounded. Then we can pass to the uniform limits in (4.13) and find a solution of the Fisher/KPP traveling wave problem. □

Exercise Compute the linearized equation of (4.28) around $u \equiv 1$ and its exponential solutions. Show that the relations for exponential decay do not bring new conditions on c compared to (4.30).

Exercise In (4.12), choose f_θ increasing in θ. Set $\zeta(v) = \frac{d}{d\theta}\tilde{w}^\theta(v)$

1. Write a differential equation for ζ.
2. Since $\zeta(v) = 0$ in $[0,\theta]$, show that $\zeta(v)$ is negative.

   Therefore, solutions of type II will never converge to solutions of Fisher/KPP equations. In practice solutions of type I do not either.

Solution $\frac{d}{dv}\zeta(v) = -\frac{df_\theta(v)}{d\theta}\,\frac{1}{\tilde{w}^\theta(v)} + \zeta(v)\frac{f_\theta(v)}{\big(\tilde{w}^\theta(v)\big)^2}.$

4.9 The Diffusive Fisher/KPP System

Another system related to the Fisher/KPP equation appears in modeling both combustion [11] and bacterial colony growth [20] (models for bacterial colony growth are treated in detail in [19]).

The so-called *Diffusive Fisher/KPP* system is

$$\begin{cases} \frac{\partial}{\partial t}u - d_u \Delta u = g(u)v, \\ \\ \frac{\partial}{\partial t}v - d_v \Delta v = -g(u)v. \end{cases} \tag{4.39}$$

Here we can take $g(u) = u^n$ for some $n \geq 1$. More generally, ignition temperature can be included with the help of a truncation function $g(\cdot) \in C^2([0,\infty))$ satisfying

$$g(0) = 0, \qquad g'(0) = 0, \qquad g'(u) > 0 \text{ for } u > 0. \tag{4.40}$$

See also Sect. 7.5.5 for related systems.

For combustion, v represents the concentration of one reactant and u the temperature. The ratio $Le := d_v/d_u$ is called the *Lewis number*.

For a bacterial colony, u represents the population density of cells (and the colony is growing) and v the nutrients consumed by the cells. See [19, 26]. The condition $g'(0) = 0$ is used to represent that bacterial multiplication is lower for isolated individuals than for communities (a type of Allee effect).

When $d_u = d_v$, a particular solution of system (4.39) consists in choosing $v = \overline{U} - u$ with $\overline{U} > 0$, a given positive number. Then it reduces to the Fisher/KPP equation (with temperature ignition in the case at hand) and thus it has traveling waves connecting $(\overline{U}, 0)$ to $(0, \overline{U})$.

In general, we claim that the traveling wave problem can always be written

$$\begin{cases} -cu' - d_u u'' = g(u)v, \qquad u(-\infty) = 1, \quad u(+\infty) = 0, \\ \\ -cv - d_v v'' = -g(u)v, \qquad v(-\infty) = 0, \quad u(+\infty) = 1. \end{cases} \tag{4.41}$$

As usual, translational invariance can be normalized by, say $u(0) = 1/2$. Notice that there are two families of steady states $(0, \overline{V})$, $(\overline{U}, 0)$, which can be connected to each other and the choice $\overline{U} = \overline{V} = 1$ seems somehow arbitrary. In fact one parameter can be normalized to 1 using a dilation on g, say $\overline{U} = 1$. Then adding up the two equations and integrating along the line, one obtains $c\ (u+v)(\infty) = c\ (u+v)(-\infty)$ and thus $\overline{V} = 1$. See Fig. 4.5.

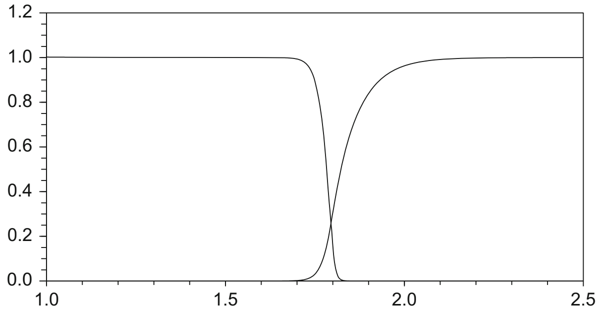

Fig. 4.5 The traveling wave profile for the Diffusive Fisher equation with $d_u = 1$, $d_v = 10$ and $g(u) = u$ in the physical space, in abscissae is x. The first unknown u has a decreasing sharp front and v a smooth increasing shape

The general study of the solutions for Lewis numbers $Le \neq 1$, is much harder than for the Fisher/KPP equation.

- Existence of a traveling wave (c, u, v) with $u' < 0$, $v' > 0$, can be found in [9] in the case of ignition temperature,
- Existence with c sufficiently large, and uniqueness, can be found in [25] in the case without ignition temperature and in the case $Le \leq 1$ with ignition temperature. A counter-example to uniqueness for $Le \geq 1$ is given in A. Bonnet [12].
- The case $Le = 0$ is also useful for many applications as nonmotile species (forest fires for example) and is treated in [24]. A more recent analysis can be found in P. Babak et al. [4].

4.10 Two Competing Species

In Sect. 1.1.3 (see Eq. (1.5)), we already mentioned the example of two species in competition for resources and competition systems. The competition between two populations with densities u_1 and u_2 is written (after normalization)

$$\begin{cases} \frac{\partial}{\partial t} u_1 - d_1 \Delta u_1 = r_1 u_1 (1 - u_1 - \alpha_2 u_2), \\ \frac{\partial}{\partial t} u_2 - d_2 \Delta u_2 = r_2 u_2 (1 - \alpha_1 u_1 - u_2). \end{cases} \tag{4.42}$$

Note that, according to Lemma 1.1 we have $u_1(t, x) \geq 0$ and $u_2(t, x) \geq 0$ when the initial data satisfy $u_1^0 \geq 0$ and $u_2^0 \geq 0$. Also the maximum principle holds: if $u_1^0 \leq 1$ then $u_1(t, x) \leq 1$, and if $u_2^0 \leq 1$ then $u_2(t, x) \leq 1$.

We may assume that species 1 is more motile than species 2, that is, $d_1 > d_2$. Depending on the predation coefficients α_1, α_2, and the specific growth rates r_1, r_2, is this an advantage? Does species 1 invade species 2 or the other way round?

We note here that there can be several steady states

- the unpopulated steady state $(0, 0)$ is always unstable,
- the one-species (monoculture) steady states are $(0,\ 1)$and $(1,\ 0)$. They are stable if $\alpha_2 > 1$ (resp. $\alpha_1 > 1$) or unstable (in fact a saddle point) if $\alpha_2 < 1$ (resp. $\alpha_1 < 1$).
- there is another homogeneous steady state defined by

$$\begin{pmatrix} 1 & \alpha_2 \\ \alpha_1 & 1 \end{pmatrix} \cdot \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

We assume that either $\alpha_2 < 1$ and $\alpha_1 < 1$ or $\alpha_2 > 1$ and $\alpha_1 > 1$, so that there is a unique positive solution, the coexistence state,

$$(U_1, U_2) = \left(\frac{1-\alpha_2}{1-\alpha_2\alpha_1}, \frac{1-\alpha_1}{1-\alpha_2\alpha_1} \right).$$

The question of invasion can now be restated so as to know which states can be connected by a traveling wave and what is the sign of the speed c of the traveling waves for $v_i(x-ct) = u_i(t,x)$. This question is relevant for instance, when $\alpha_1 > 0$ and $\alpha_2 > 0$ and one wishes to connect the two stable states $(1,\ 0)$ and $(0,\ 1)$

$$\begin{cases} -cv_1' - d_1 v_1'' = v_1(1 - v_1 - \alpha_2 v_2), \\ -cv_2' - d_2 v_2'' = v_2(1 - \alpha_1 v_1 - v_2), \\ v_1(-\infty) = 1, \quad v_2(-\infty) = 0, \qquad v_1(+\infty) = 0, \quad v_2(+\infty) = 1. \end{cases}$$

This question is treated in [31], in Lewis et al. [23] and the front dynamic is treated in G. Barles et al. [6], Barles and Souganidis [5], and W. Fleming and P.E. Souganidis [16]. See also Sect. 7.6.1 for Turing instability.

Exercise Consider the associated O.D.E system. Prove that

1. when $\alpha_1 < 1$ and $\alpha_2 < 1$, the coexistence steady states U_1 and U_2 are less than 1 and are stable,
2. when $\alpha_1 > 1$ and $\alpha_2 > 1$, the steady states U_1 and U_2 are less than 1 and are unstable.
3. Find a, b, c such that the quantity $E = au_1 + bu_2 - c\ln(u_1) - \ln(u_2)$ satisfies, for some real numbers λ, μ, ν

$$\frac{d}{dt}E(t) = -\big(\lambda + \mu u_1(t) + \nu u_2(t)\big)^2.$$

4. Derive from this equality the long term behavior of the system.

Solution We only solve the stability questions. The linearized matrix around (U_1, U_2) is given by

$$L = \begin{pmatrix} -r_1 U_1 & -\alpha_2 r_1 U_1 \\ & \\ -\alpha_1 r_2 U_2 & -r_2 U_2 \end{pmatrix}$$

and $\mathrm{tr}(L) = -(r_1 U_1 + r_2 U_2) < 0$, $\det(L) = r_1 r_2 U_1 U_2 (1 - \alpha_1 \alpha_2)$. Therefore we have

1. For $\alpha_1\alpha_2 < 1$, $\det(L) > 0$ and the two eigenvalues have a negative real part. The system is stable.

2. For $\alpha_1\alpha_2 > 1$, $\det(L) < 0$ and one of the two eigenvalues are real and one is positive (thus unstable) and the other is negative.

Exercise (Potential Case) Consider the system of two competing species (all the coefficients are positive)

$$\begin{cases} \frac{\partial}{\partial t}u - d_u\Delta u = r_1 u(1 - 2av^2 - u), & t \geq 0,\ x \in \mathbb{R}, \\ \frac{\partial}{\partial t}v - d_v\Delta v = r_2 v(1 - 2bu^2 - v). \end{cases}$$

This system has (among others) two steady states $(1,\ 0)$ and $(0,\ 1)$.

1. Write the equation for a traveling wave with velocity c that connects these two states.
2. Compute the value of $\gamma > 0$ such that there is a function $P(u, v)$ such that

$$r_1 u(1 - 2av^2 - u)\frac{du}{dx} + r_2 v(1 - 2bu^2 - v)\frac{\gamma\, dv}{dx} = \frac{d}{dx}P(u, v)$$

for all regular functions $u(x)$ et $v(x)$, $x \in \mathbb{R}$.
3. Compute the sign of the speed c as a function of a and b.
4. What is the ecological interpretation.

Solution

1. For $x \in \mathbb{R}$,

$$\begin{cases} -cu' - d_u u'' = r_1 u(1 - 2av^2 - u), & u(-\infty) = 1, \quad v(-\infty) = 0, \\ -cv' - d_v v'' = r_2 v(1 - 2bu^2 - v), & u(\infty) = 0, \quad v(-\infty) = 1. \end{cases}$$

2. $\gamma = \frac{r_1 a}{r_2 b}$. $P(u, v) = r_1 u - r_1 a u^2 v^2 - r_1 \frac{u^2}{2} + \gamma r_2 v - \gamma \frac{r_2}{2} v^2$.
3. We compute following Sect. 4.1

$$-c \int [(u')^2 + (v')^2] + 0 = \int u'[r_1 u(1 - 2av^2 - u)] + v'[r_2 v(1 - 2bu^2 - v)] =$$
$$= \int \frac{dP}{dx} + P(0, 1) - P(1, 0) = \frac{r_1}{2}(\frac{a}{b} - 1).$$

So that c has the sign of $b - a$.
4. This system represents two species competing for space, with a carrying capacity normalized to 1. Independently of the reproduction rate, the species that occupies more of the other niche will invade space.

4.11 Reid's Paradox

It is not always easy to apply the theory of traveling waves to real problems arising in ecology. A famous example is Reid's paradox (1899).

At the end of the last glacial age, 10–15,000 years ago, recolonization of continents by trees and plants occurred. Records show that the front followed closely the withdrawal of glaciers. This corresponds to a migration speed far too high for the dispersal capabilities of seeds. The explanation of this observation is still an open problem in ecology.

A possible explanation [30] is the long distance dispersal effect by other species (birds and humans that could take seeds far away from the trees). A mathematical framework to quantify these effects can be found in Kot et al. [22] and uses the formalism of Sect. 4.10.

Another explanation is diffusion and growth proceeding from cryptic populations. Fossil records indeed indicate that small refuges existed [7]. Mathematical analysis can be found in Roques et al. [29].

References

1. Allee, W.C.: Animal Aggregations: A Study in General Sociology. University of Chicago Press, Chicago (1931)
2. Allen, S.M., Cahn, J.W.: A macroscopic theory for antiphase boundary motion and its application to antiphase domain coarsening. Acta Metall. **270**, 1085–1095 (1979)
3. Aranson, D.G., Weingerger, H.F.: Nonlinear diffusion in population genetics, combustion, and nerve pulse propagation. In: Lecture Notes in Mathematics, vol. 446, pp. 5–49. Springer, Berlin/Heidelberg (1975)
4. Babak, P., Bourlioux, A., Hillen, T.: The effect of wind on the propagation of an idealized forest fire. SIAM J. Appl. Math. **70**(4), 1364–1388 (2009)
5. Barles, G., Souganidis, P.E.: Front propagation for reaction-diffusion equations arising in combustion theory. Asymptot. Anal. **14**, 277–292 (1997)
6. Barles, G., Evans, L.C., Souganidis, P.E.: Wavefront propagation for reaction diffusion systems of PDE. Duke Math. J. **61**, 835–858 (1990)
7. Benett, K.D., Provan, J.: What do we mean by 'refugia'? Quat. Sci. Rev. **27**, 2449–2455 (2008)
8. Berestycki, H., Hamel, F.: Reaction-Diffusion Equations and Propagation Phenomena (book in preparation)
9. Berestycki, H., Nicolaenko, B., Scheurer, B.: Traveling wave solutions to combustion models and their singular limits. SIAM J. Math. Anal. **16**(6), 1207–1242 (1985)
10. Berestycki, H., Nadin, G., Perthame, B., Ryzhik, L.: The non-local Fisher-KPP equations: traveling waves and steady states. Nonlinearity **22**, 2813–2844 (2009)
11. Billingham, J., Needham, N.L.: The development of travelling waves in quadratic and cubic autocatalysis with unequal diffusion rates, I. Permanent form travelling waves. Philos. Trans. R. Soc. Lond. A **334**, 1–24 (1991)
12. Bonnet, A.: Non-uniqueness for flame propagation when Lewis number is less than 1. Eur. J. Appl. Math. **6**, 287–306 (1995)
13. Evans, J.: Nerve axon equations 4: the stable and unstable impulse. Indiana Univ. Math. J. **24**(12), 1169–1190 (1975)

14. Fife, P.C.: Mathematical Aspects of Reacting and Diffusing Systems. Lecture Notes in Biomathematics, vol. 28. Springer, Berlin (1979)
15. Fisher, R.A.: The Genetical Theory of Natural Selection. Clarendon Press, Oxford (1930). Deuxième éd., Dover (1958). Troisième édition, présentée et annotée par Henry Bennett, Oxford University Press (1999)
16. Fleming, W.H., Souganidis, P.E.: PDE-viscosity solution approach to some problems of large deviations. Ann. Scuola Norm. Sup. Pisa Cl. Sci. **4**, 171–192 (1986)
17. Françoise, J.-P.: Oscillations en biologie. Collection Mathématiques et Applications. SMAI, Springer, Paris (2005)
18. Garnier, J., Giletti, T., Hamel, F., Roques, L.: Inside dynamics of pulled and pushed fronts. J. Math. Pures Appl. **98**(4), 428–449 (2012)
19. Golding, I., Kozlovski, Y., Cohen, I., BenJacob, E.: Studies of bacterial branching growth using reaction-diffusion models for colonial development. Physica A **260**, 510–554 (1998)
20. Kessler, D.A., Levine, H.: Fluctuation induced diffusive instabilities. Nature **394**, 556–558 (1998)
21. Kolmogorov, A.N., Petrovski, I.G., Piskunov, N.S.: Étude de l'équation de la diffusion avec croissance de la quantité de matière et son application à un problème biologique. Bulletin Université d'État de Moscou (Bjul. Moskowskogo Gos. Univ.), Série internationale **A1**, 1–26 (1937)
22. Kot, M., Lewis, M.A., Van der Driessche, P.: Dispersal data and the spread of invading organisms. Ecology **77**(7), 2027–2041 (1996)
23. Lewis, M.A., Li, B., Weinberger, H.F.: Spreading speed and linear determinacy for two-species competition models. J. Math. Biol. **45**, 219–233 (2002)
24. Logak, E., Loubeau, V.: Travelling wave solutions to a condensed phase combustion model. Asymptot. Anal. **12**(4), 259–294 (1996)
25. Marion, M.: Qualitative properties of a nonlinear system for laminar flames without ignition temperature. Nonlinear Anal. **9**(11), 1269–1292 (1985)
26. Mimura, M., Sakaguchi, H., Matsuchita, M.: Reaction diffusion modeling of bacterial colony patterns. Physica A **282**, 283–303 (2000)
27. Nadin, G., Perthame, B., Tang, M.: The non-local Fisher-KPP equation: traveling waves and steady states. Can a traveling wave connect two unstable states? The case of the non-local Fisher equation. C. R. Acad. Sci. Paris Ser. I **349**, 553–557 (2011)
28. Okubo, A., Levin, S.A. (eds.): Diffusion and Ecological Problems, Modern Perspectives, 2nd edn. Springer, New York (2001)
29. Roques, L., Hamel, F., Fayard, J., Fady, B., Klein, E.K.: Recolonisation by diffusion can generate increasing rates of spread. Theor. Popul. Biol. **77**, 205–212 (2010)
30. Skellam, J.G.: Random dispersal in theoretical populations. Biometrika **38**(1/2), 196–218 (1951)
31. Volpert, A.I., Volpert, V.A.: Traveling Wave Solutions of Parabolic Systems. Translation of Mathematical Monographs, vol. 140. AMS, Providence (1994)
32. Zel'dovich, Y.B., Frank-Kamenetskii, D.A.: The theory of thermal flame propagation. Zhur. Fiz. Khim. **12**, 100 (1938) (in Russian)

Chapter 5
Spikes, Spots and Pulses

Typical behavior of solutions of elliptic equations or systems are *spikes*. These are solutions that vanish at plus and minus infinity. In higher dimensions these are also called spots, which are typical Turing patterns. In parabolic systems, solutions that vanish at both ends also occur and they travel with constant speed: we call them *pulses*, while the traveling waves that we encountered in Chap. 4 take different values at each end. We give several examples from different areas of biology, an illustration is Fig. 5.1.

5.1 Spike Solutions

5.1.1 A Model for Chemotaxis

We refer to [3, 6, 16, 22, 23] for introductions to the complex subject of chemotaxis. Here we consider a very particular question.

Consider a density $u(x)$ of bacteria attracted by a chemoattractant whose concentration is denoted by $v(x)$. Following [7], the variant of the Keller-Segel model that we use takes into account the nonlinear diffusion of cells and we introduce an exponent p in the diffusion term. In the modeling literature, nonlinear diffusion represents saturation effects in high density regions (volume filling, quorum sensing) and can be derived from refined models at the mesoscopic (kinetic) or even microscopic (individually centered) scales, [26].

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_5

Fig. 5.1 Example of spots in nature; a zoom on an orchid flower

Also we only consider a one space dimension in order to carry out explicit calculations,

$$\begin{cases} -(u^{1+p})_{xx} + (\chi u v_x)_x = 0, \qquad x \in \mathbb{R}, \\ -v_{xx} + \alpha v = u, \\ u(-\infty) = v(-\infty) = u(\infty) = v(\infty) = 0. \end{cases} \tag{5.1}$$

We are going to prove the following result

Proposition 5.1 *Assume that* $0 < p < 1$*, then the system* (5.1) *has a unique spike solution which attains its maximum at* $x = 0$ *and satisfies* $u \geq 0$*,* $v \geq 0$.

Proof First Step (Reduction to a Single Equation) Solution u can be obtained explicitly in terms of v, writing $(u^{1+p})_x = \chi u v_x$ (the constant vanishes because we expect that u, v and their derivatives vanish at $\pm\infty$). This is also, and for the same reason

$$(u^p)_x = \frac{p\chi}{1+p} v_x, \qquad u = \left(\frac{p\chi}{1+p} v\right)^{1/p}.$$

We may insert this expression in the equation for v, which gives

$$-v_{xx} + \alpha v = \left(\frac{p\chi}{1+p} v\right)^{1/p}. \tag{5.2}$$

One can solve explicitly this type of equation. We multiply by v_x and find

$$-\Big(\frac{(v_x)^2}{2}\Big)_x + \alpha\Big(\frac{(v)^2}{2}\Big)_x = \frac{1}{2}\big(g(v)\big)_x, \qquad v(-\infty) = v(\infty) = 0,$$

with $g(v) = \frac{2p}{1+p}\left(\frac{p\chi}{1+p}\right)^{1/p} v^{1+1/p}$. Therefore, we have (the integration constant still vanishes because of the behavior at infinity)

$$(v_x)^2 = \alpha v^2 - g(v). \tag{5.3}$$

2nd Step (Resolution of the Reduced Equation) We now choose to normalize the translation invariance so that v attains its maximum at $x = 0$ and define $v(0) = v_0 > 0$. Then we should have $g(v_0) = \alpha v_0^2$ because at a maximum point $v_x(0) = 0$. This defines the unique value v_0 because of the assumption for p. For $v \leq v_0$, we have $\alpha v^2 - g(v) \geq 0$ and for $v > v_0$, we have $\alpha v^2 - g(v) < 0$. Thus, we can determine the correct sign for the square root in Eq. (5.3). We find

$$\begin{cases} v_x(x) = -\sqrt{\alpha v(x)^2 - g\big(v(x)\big)}, & v(0) = v_0, \quad x > 0, \\ v_x(x) = \sqrt{\alpha v(x)^2 - g\big(v(x)\big)}, & v(0) = v_0, \quad x < 0. \end{cases}$$

This defines a unique function $v(x)$, which converges to 0 as $x \to \pm\infty$. □

One can prove that the evolution equation associated with (5.1) has the following behavior. If its initial data satisfies $\int_{\mathbb{R}} u^0(x)dx < \int_{\mathbb{R}} u(x)dx$ then $u(t,x) \to 0$ as $t \to \infty$. If its initial data satisfies $\int_{\mathbb{R}} u^0(x)dx > \int_{\mathbb{R}} u(x)dx$ then $u(t,x)$ blows-up (see Chap. 6) in finite time and concentrates as a Dirac mass. See [7].

Exercise What happens when $p = 1$ in the above calculation? Are there still spike solutions?

Exercise Compute how the solution v to (5.1) decays to 0 at infinity. Prove that u satisfies $\int_{\mathbb{R}} u(x)dx < \infty$.

Exercise Consider the general chemotaxis model

$$\begin{cases} -(u^{1+p})_{xx} + \big(u^q v_x\big)_x = 0, & x \in \mathbb{R}, \\ -v_{xx} + \alpha v = u^r. \end{cases}$$

For which range of positive parameters p, q, r are there spike solutions?

5.1.2 A Non-local Model from Adaptive Evolution

Non-local equations also create concentration effects leading to spikes. We take an example from the theory of adaptive evolution. A population is structured by a physiological parameter (denoted by x below). This parameter could represent the size of an organ of the individuals, a proportion of resources used for growth and multiplication, or any relevant phenotypical parameter, useful to describe the adaptation of the individuals, i.e., their ability to use the nutrients for reproduction. See Diekmann [10] and F. Chalub and J.-F. Rodriguez [8].

We denote by $u(t,x)$ the density of individuals with trait $x \in \mathbb{R}$; the simplest model is to write that each trait corresponds to a different birth rate. We assume that the total population, whatever the individual traits, compete and contribute and increase the death rate

$$\begin{cases} \frac{\partial}{\partial t} v(t,x) - D\Delta v = v\big(b(x) - \varrho(t)\big), & t \geq 0,\ x \in \mathbb{R}, \\ \varrho(t) = \int_{\mathbb{R}} v(t,x)dx, \\ v(t=0,x) = v^0(x) \geq 0. \end{cases} \tag{5.4}$$

The Laplacian term Δv takes into account mutations (it should be included in the birth term, but we choose here to simplify the equation as much as possible), $b(x)$ is the birth rate depending on the trait x. Finally, $-\varrho$ represents the death term, as in the Fisher/KPP equation, with the main difference that the total population is used for this quadratic death term.

We now look for a steady state solution of this model that vanishes at $\pm\infty$ so as to find a spike solution

$$\begin{cases} -Du''(x) = u(x)\ \big(b(x) - \overline{\varrho}\big), & x \in \mathbb{R}, \\ \overline{\varrho} = \int_{\mathbb{R}} u(x)dx, \qquad u(x) > 0, \\ u(\pm\infty) = 0. \end{cases} \tag{5.5}$$

The problem (5.5) has a simple interpretation. One first solves the eigenvalue ϱ of the PDE in (5.5); then the total density constraint is simply a normalization of the eigenfunction. Therefore, its solution follows from the Krein-Rutman theorem (Perron-Froebenius theory in infinite dimension). The spike phenomena is well-known for a small diffusion $D \approx 0$; in quantum mechanics, it is called the *Anderson localization*. This can be analyzed conveniently using asymptotic analysis related to Hamilton-Jacobi equations [4]. The solution exists with quite general assumptions for b. We show in Fig. 5.2 two solutions for $D = 0, 1$ and $D = 0.01$ for the bimodal birth rate

$$b(x) = \frac{1}{(1 + 50(x - 15)^2)^{10}} + \frac{.9}{(1 + 50(x - 85)^2)^5}.$$

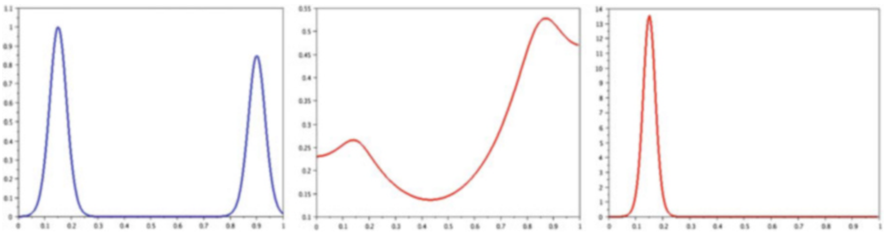

Fig. 5.2 One and two spike solutions $u(x)$ of Eq. (5.5) for the birth rate $b(x)$ plotted on the *left*. The figure in the *center* is $D = 0.1$ and the figure on the *right* is $D = 0.01$. This shows the localization effect resulting from small diffusion. Abscissae are x

As a theoretical result we build a simple example with an explicit solution that explains the existence of a spike solution

Theorem 5.2 *Assume $b(x)$ has the form*

$$b(x) = \begin{cases} b_- > 0 & \text{for } |x| > a, \\ b_+ > b_- & \text{for } |x| < a, \end{cases}$$

then there is a unique spike solution of (5.5), and it is single spiked.

Theorem 5.3 *Assume that there is a constant C_0 such that $0 \le v^0 \le C_0 u$, then the solution of (5.4) converges as $t \to \infty$ to the steady state solution of (5.5).*

Proof of Theorem 5.2 We first consider a solution, forgetting the condition $\overline{\varrho} = \int u$ and find an intrinsic condition for $\overline{\varrho}$. For $x \le -a$ the equation is $-u''(x) = u(x)(b_- - \overline{\varrho})$ and the conditions $u > 0$ and $u(-\infty) = 0$ impose $\overline{\varrho} > b_-$ to give the explicit solution

$$u(x) = \mu_- e^{\lambda_- x}, \qquad x \le -a, \qquad \lambda_- = \sqrt{\overline{\varrho} - b_-}.$$

Similarly, we have

$$u(x) = \mu_+ e^{-\lambda_- x}, \qquad x \ge a.$$

In order to connect these two branches, we require that $\overline{\varrho} < b_+$ and

$$u(x) = \mu_1 \cos(\lambda_0 x) + \mu_2 \sin(\lambda_0 x), \qquad -a \le x \le a, \qquad \lambda_0 = \sqrt{b_+ - \overline{\varrho}}.$$

The sign condition $u(x) > 0$ also imposes $\mu_1 > 0$ (at $x = 0$) and $\lambda_0 a < \pi/2$ (otherwise take $\lambda_0 x_0 = \pm\pi/2$).

Now, we have to check the continuity of u and u' at the points $\pm a$. This gives the conditions

$$\begin{cases} \mu_- e^{-\lambda_- a} = \mu_1 \cos(\lambda_0 a) - \mu_2 \sin(\lambda_0 a), \\ \mu_+ e^{-\lambda_- a} = \mu_1 \cos(\lambda_0 a) + \mu_2 \sin(\lambda_0 a), \end{cases}$$

$$\begin{cases} \mu_- \lambda_- e^{-\lambda_- a} = \mu_1 \lambda_0 \sin(\lambda_0 a) + \mu_2 \lambda_0 \cos(\lambda_0 a), \\ \mu_+ \lambda_- e^{-\lambda_- a} = \mu_1 \lambda_0 \sin(\lambda_0 a) - \mu_2 \lambda_0 \cos(\lambda_0 a). \end{cases}$$

From these equalities we deduce first that the quantity $\mu = \frac{1}{2}(\mu_- + \mu_+)$ satisfies

$$\begin{cases} \mu e^{-\lambda_- a} = \mu_1 \cos(\lambda_0 a), \\ \mu \lambda_- e^{-\lambda_- a} = \mu_1 \lambda_0 \sin(\lambda_0 a), \end{cases}$$

consequently, $\lambda_- = \lambda_0 \tan(\lambda_0 a)$. In other words the parameter $\overline{\varrho}$ should satisfy

$$b_- \le \overline{\varrho} \le b_+, a\sqrt{b_+ - \overline{\varrho}} < \pi/2, \qquad \sqrt{\overline{\varrho} - b_-} = \sqrt{b_+ - \overline{\varrho}}\ \tan(a\sqrt{b_+ - \overline{\varrho}}).$$

By monotonicity we see that there is a unique $\overline{\varrho}$ satisfying these conditions, and that knowing μ, then μ_1 follows by proportionality to μ.

Next, we go back to the four conditions and now find

$$\begin{cases} \frac{\mu_+ - \mu_-}{2} e^{-\lambda_- a} = \mu_2 \sin(\lambda_0 a), \\ \frac{\mu_+ - \mu_-}{2} \lambda_- e^{-\lambda_- a} = -\mu_2 \lambda_0 \cos(\lambda_0 a), \end{cases}$$

and straightforward sign considerations show that $\mu_2 = 0$ and $\mu_- = \mu_+$.

Therefore, we have the only free parameter μ left. We use it to enforce the mass condition $\overline{\varrho} = \int_{\mathbb{R}} u(x)dx$ and thus we have indeed a unique solution. □

Proof of Theorem 5.3 Consider the solution $\tilde{v}(t,x) \ge 0$ to the heat equation

$$\begin{cases} \frac{\partial}{\partial t}\tilde{v}(t,x) - \Delta \tilde{v} = \tilde{v}\big(b(x) - \overline{\varrho}\big), \qquad t \ge 0,\ x \in \mathbb{R}, \\ \tilde{v}(t=0,x) = v^0(x). \end{cases} \tag{5.6}$$

This is a heat equation with 0 the first eigenvalue of the steady equation. We know from the maximum principle that $0 \le \tilde{v}(t,x) \le C_0 u(x)$ (see the proof of lemma). And from the general theory of dominant eigenvectors of positive operators (Krein-Rutman theorem and relative entropy [23])

$$v(t,x) \xrightarrow[t\to\infty]{} \lambda u(x),$$

for some $\lambda \in \mathbb{R}$.

On the other hand we can look for the solution of (5.4) with the form $v(t,x) = \mu(t)\tilde{v}(t,x)$ with $\mu(t) \ge 0$. We have

$$\frac{\partial}{\partial t} v(t,x) - \Delta v - v\big(b(x) - \varrho(t)\big) = \dot{\mu}(t)\tilde{v}(t,x) + \mu(t)\tilde{v}(t,x)\big(\varrho(t) - \overline{\varrho}\big),$$

which allows us to find $\mu(t)$ by the equation

$$\dot{\mu}(t) + \mu(t)\big(\varrho(t) - \overline{\varrho}\big) = 0.$$

But we have $\varrho(t) = \int_{\mathbb{R}} v(t,x)dx = \mu(t)\int_{\mathbb{R}} \tilde{v}(t,x)dx = \mu(t)\lambda(t)$, with

$$\lambda(t) = \int_{\mathbb{R}} \tilde{v}(t,x)dx \xrightarrow[t\to\infty]{} \lambda.$$

Finally, we obtain

$$\begin{cases} \dot{\mu}(t) + \mu(t)\big(\mu(t)\lambda(t) - \overline{\varrho}\big) = 0, \\ \mu(0) = 1. \end{cases}$$

The solution satisfies

$$\mu(t) \xrightarrow[t\to\infty]{} \overline{\varrho}/\lambda.$$

This is exactly the anticipated result. □

Exercise Consider the model

$$\begin{cases} \frac{\partial}{\partial t} v(t,x) - \Delta v = v\big(\frac{b(x)}{1+\varrho(t)} - d(x)\varrho(t)\big), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \varrho(t) = \int_{\mathbb{R}} v(t,x)dx. \end{cases} \tag{5.7}$$

Assume that b, d still take two different values (with same discontinuity points) and gives a condition for existence of a single spike solution.

5.2 Traveling Pulses

We describe the mathematical mechanism for creating *pulses*, which means spikes that are moving as traveling waves. The most famous example, namely the Hodgkin-Huxley system, describes accurately the propagation of an ionic/electric signal along nerves. The Hodgkin-Huxley system is rather complex and we prefer here to retain only simplified models, which we hope, explain better the mechanism.

5.2.1 Fisher/KPP Pulses

A method to generate a pulse from the Fisher/KPP equation is to include a component $v(t,x)$, which drives the state $u = 1$ back to zero. This arises with a certain delay because this component v has to increase from zero (a state we impose initially) to a quantity larger than 1 so as to ensure that u itself decreases to zero. With these considerations, we arrive to the system

$$\begin{cases} \frac{\partial}{\partial t} u(t,x) - \Delta u = u[1 - u - v] \\ \qquad \frac{\partial}{\partial t} v(t,x) = u, \end{cases} \tag{5.8}$$

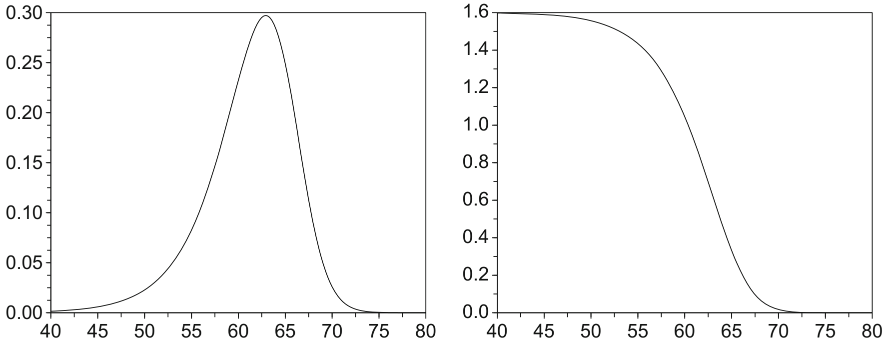

Fig. 5.3 Fisher/KPP pulses, these are traveling wave solutions of the system (5.8). The solution is presented as a function of x (abscissae), at a given time. The pulse propagates from left to right. *Left*: $u(t,x)$ exhibits a pulse shape, i.e., it vanishes at both endpoints. *Right*: $v(t,x)$ is a traveling wave as in the Fisher/KPP equation but it does not have a pulse shape (in opposition to the FitzHugh-Nagumo system)

The solutions at a given time are depicted in Fig. 5.3. One can observe that u is indeed a pulse but v does not vanish at $x = -\infty$ in opposition with the FitzHugh-Nagumo system.

5.2.2 FitzHugh-Nagumo System

Several parabolic models have been used in neurosciences for the propagation of nerve impulses. In the 1950s, the model proposed by Hodgkin and Huxley gave particularly accurate results when compared to experimental results along the giant squid axon (see [12, 22]). This model has stimulated the development of theories for electrophysiology, cardiac, neural communications by electrical signaling or neural rhythms.

The FitzHugh-Nagumo system is nowadays the simplest model used to describe pulse propagations in a spatial region. We give two versions, one for electric potential, one for calcium waves.

The simpler and original system is

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - \varepsilon\Delta u = \frac{1}{\varepsilon}[u(1-u)(u-\alpha) - v], \\ \\ \frac{\partial}{\partial t}v(t,x) = \gamma u - \beta v, \end{cases} \tag{5.9}$$

in particular, we have included the small parameter ε responsible for the slow-fast dynamic.

In Fig. 5.4 (Left) we depict a pulse traveling with parameters indicated in the figure legend. We choose here $\alpha < 0.5$ in order to propagate a traveling wave in the Allen-Cahn equation for u (initially $v \equiv 0$). This switches on the equation for

v, and with a certain delay it inhibits the pulse and u goes back to the other stable value, $u = 0$. For that we require the condition

$$u(1-u)(u-\alpha) < \frac{\gamma}{\beta}u \quad \text{for } 0 < u < 1.$$

In the other case we can reach an equilibrium $\beta v = \gamma u$, which transforms the bistable nonlinearity into a monostable nonlinearity.

The parameter ε controls the stiffness of the fronts, β the width of the pulse and $\frac{\gamma}{\beta}$ the type of wave.

As one can see in Fig. 5.4, the solution u can reach negative values. This is in accordance with electrical potential waves. This can be seen as a modeling error for concentration waves. Also the shape of the 'polarization wave' does not always fit with experimental observations (for example for cardiac electric waves). This is the reason why several variants exist.

A possible way to guarantee that u remains nonnegative is to modify the FitzHugh-Nagumo system into

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - \varepsilon\Delta u = \frac{1}{\varepsilon}u[(1-u)(u-\alpha) - v], \\ \\ \qquad\qquad \frac{\partial}{\partial t}v(t,x) = v_\infty(u) - v, \end{cases} \tag{5.10}$$

where $v_\infty(\cdot)$ represents the equilibrium on v in the potential (concentration) u. The choice of this nonlinear function allows for more generality.

- For $v_\infty(u) = ku$, the system is due to J.M. Roger and A.D. McCulloch [25].
- For $v_\infty(u) = ku(u-1-a)$, the system is called Aliev-Panfilov [2].

Figure 5.5 shows a pulse for Eq. (5.10) with $\alpha = 0.2$, $v_\infty(u) = 3. * (u-0.4)_+$ (here the numbers are adapted to $\alpha = 0.2$) which propagates from left to right. Two values of ε are represented.

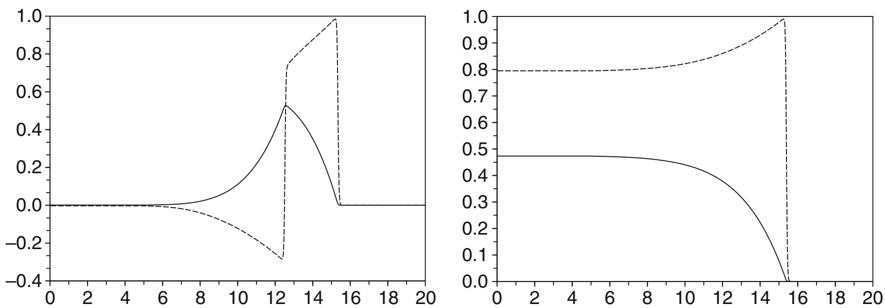

Fig. 5.4 Solutions of the FitzHugh-Nagumo equation (5.9) with $\varepsilon = 0.02$, $\alpha = 0.1$ and $\beta = .2$ and (*Left*) $\gamma = .25*\beta$, (*Right*) $\gamma = .15*\beta$. According to the explanation in the text, for γ large we obtain a traveling pulse, for γ small we obtain a traveling wave. *Dashed line* is u, *continuous line* is v (amplified by a factor 4). See also Fig. 5.5. The original Fitz-Hugh Nagumo system exhibits an undershoot of u, which is observed in neurones and is called hyperpolarization

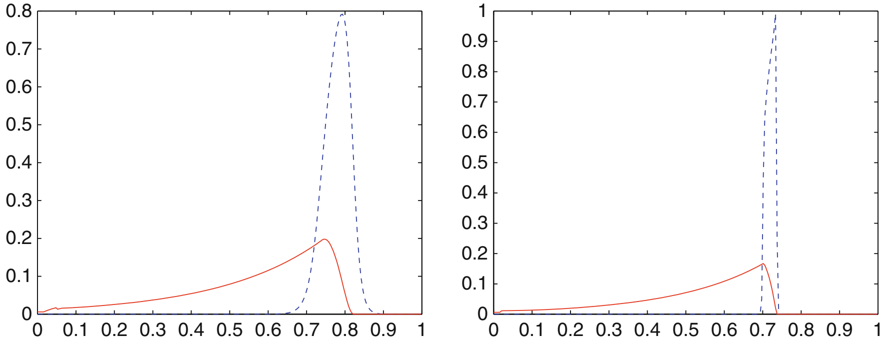

Fig. 5.5 Solutions of the space structured FitzHugh-Nagumo system (5.10) with $\alpha = 0.2$ and $\varepsilon = 0.01$ (*left*), $\varepsilon = 0.001$ (*right*); we represent both $u(t,x)$ (*dashed line*) and $v(t,x)$ (*continuous line*) as a function of x, at a given time. The pulse propagates from left to right

5.3 Unstable Waves and Dynamic Patterns

Higher dimension traveling waves or pulses can become unstable and generate dynamic patterns. The paper [14] describes the steps for including biophysical phenomena of increasing complexity, all producing instabilities. Their approach is applied to bacterial colony growth. Applications to cancer modeling, and analysis of the range of parameters to obtain instabilities, has been developed by M. Ben Amar and co-authors [5, 9].

5.3.1 The Gray-Scott System (1)

The mechanism that generates unstable traveling waves has been observed in chemical reactions and a typical model is the Gray-Scott system. In the simplest case (see the extension in (7.20)), the Gray-Scott system is written as

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u^2 v - Au, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = -u^2 v, \\ \dfrac{\partial w}{\partial t} = Au. \end{cases} \tag{5.11}$$

Here u denotes the concentration of a component that reacts with v (and consumes it) and also generates a component w.

System (5.11) generates already very complex solutions which exhibit beautiful dynamic patterns. Examples are shown in Figs. 5.6 and 5.7. One can observe that the first component $u(t,x)$ exhibits a pulse shape that propagates outward. The

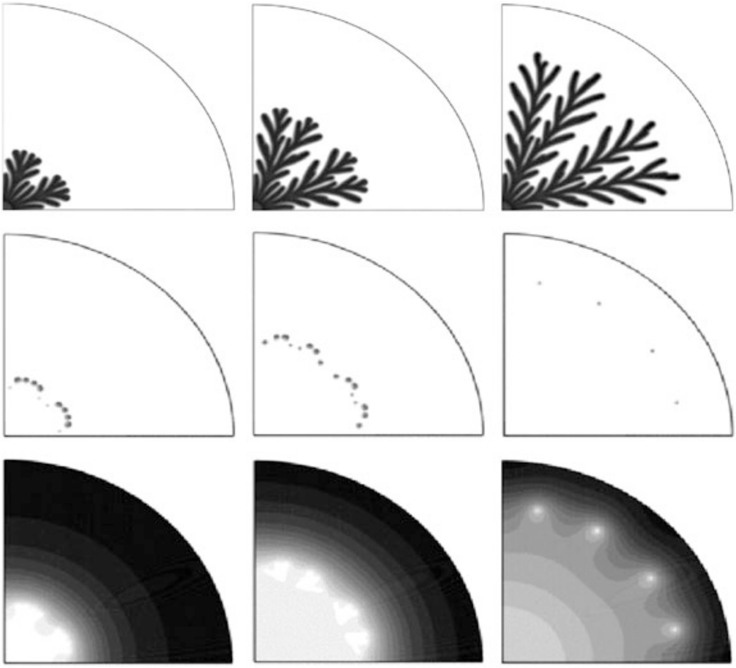

Fig. 5.6 Three snapshots of a simulation of the Gray-Scott system (5.11) with an unstructured grid showing how an unstable radial wave generates a pattern. *Upper figures*: the quantities w. *Middle*: the quantity $u(x,t)$. *Lower figures*: the quantity v. Computations by A. Marrocco using a mixed finite element method. Taken from A. Marrocco et al. (2010). Models of Self-Organizing Bacterial Communities and Comparisons with Experimental Observations. Mathematical modeling of Natural Phenomena, 5 (01), pp 148–162. doi:10.1051/mmnp/20105107. Available at http://www.mmnp-journal.org/

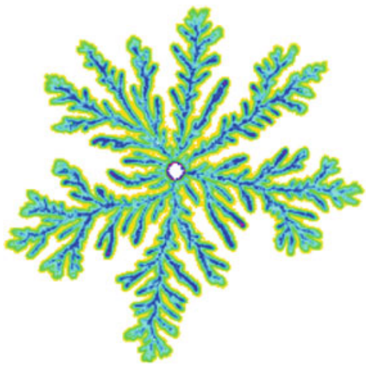

Fig. 5.7 Another simulation (with different parameters) of the Gray-Scott system (5.11) with an unstructured grid: the quantity w is depicted. Courtesy of S.M. Kaber, computations using the software FreeFEM++ [13, 15]

component $v(t,x)$ resembles a more conventional, radially symmetric traveling wave. The 'burnt' byproduct $w(t,x)$ exhibits a dentritic dynamic pattern that results from the localization effect on u.

An analysis of scales in this problem and of the concentration effect can be found in T. Kolokolnikov et al. [18], C. Muratov and V.V. Ospinov [21]. For the Schnakenberg variant, see Sect. 7.5.6, the authors arrive to fast reaction/small diffusion scales written

$$\begin{cases} \dfrac{\partial u}{\partial t} - \varepsilon^2 \Delta u \quad = u^2 v - u, \\ \varepsilon^2 \dfrac{\partial v}{\partial t} - d_v \Delta v = a - \frac{u^2 v}{\varepsilon^2}. \end{cases}$$

5.3.2 The Mimura System for Bacterial Colony

Bacterial colonies also often exhibit remarkable patterns, see Figs. 5.8 and 5.9. They follow from complex and poorly understood collective interactions between cells due to several effects: random motion of the individual cells, cell multiplication and colony expansion, release of various signaling molecules in their environment resulting, e.g., in promoting chemoattraction (chemotaxis) or in modifying surface tension. The patterns depend heavily on the type of bacteria and on the support used for the experiment (solid, semi-solid, liquid) and its nutrient content. A good account on these issues can be found in [14, 22].

A simple model for the expansion of dentritic colonies is due to Mimura [19]. It takes into account only three simple effects: (i) Brownian motion of active cells whose population density is denoted by $n(t,x)$ below, (ii) a nutrient concentration

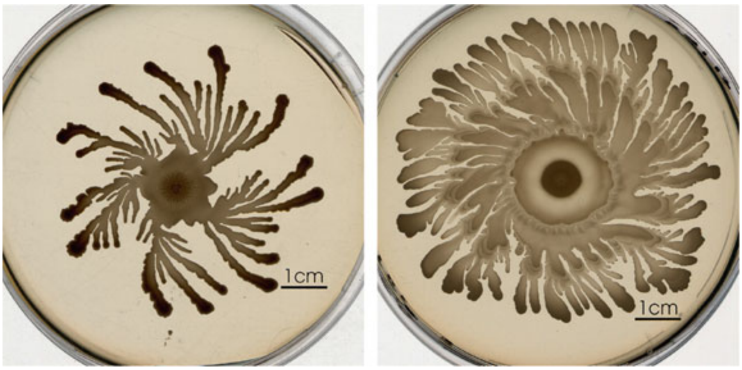

Fig. 5.8 Bacterial colony patterns of *Bacillus subtilis* 168 grown on LB solid medium (*left*) and LB semi-solid medium (*right*). Experiments by Simone Séror and Barry Holland, Institut de Génétique et Microbiologie, Université Paris-Sud. Courtesy of the authors, © S. Séror. The diameter of these swarming patterns is around 9 cm; the bacteria were inoculated in the center and multiply and move radially in approximately 24 h

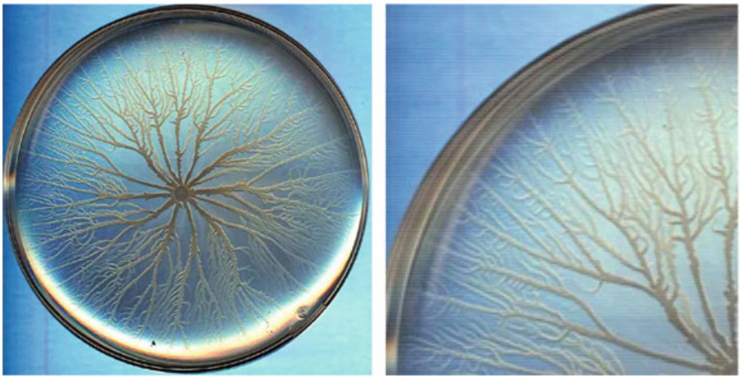

Fig. 5.9 A highly dentritic swarming colony of *Bacillus subtilis* 168 (a strain producing a surfactant) by Simone Séror and Barry Holland after 24 h swarming on B-medium (three times slower growth than on LB medium). From A. Marrocco, H. Henry, I.B. Holland, M. Plapp, S.J. Séror and B. Perthame (2010). Models of Self-Organizing Bacterial Communities and Comparisons with Experimental Observations. Mathematical modeling of Natural Phenomena, 5 (01), pp 148–162. doi:10.1051/mmnp/20105107. Available at http://www.mmnp-journal.org/

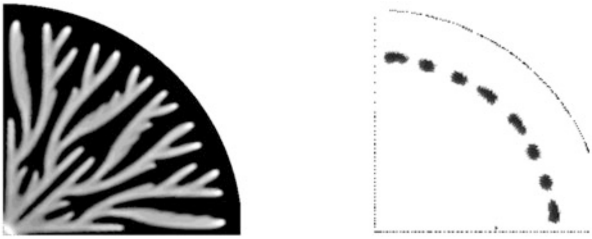

Fig. 5.10 Solutions given by the Mimura system (5.12) at a fixed time. *Left*: frozen bacteria $f(t,x)$. *Right*: active bacteria $n(t,x)$. Computations by A. Marrocco

$c(t,x)$, which diffuses in the medium and is consumed by the active cells for growth, (iii) the active cells become frozen proportionally to n and then they do not move. The specific form of the equations proposed by Mimura are given in system (5.12) and numerical results are presented in Figs. 5.10 and 5.11.

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - d_1 \Delta n(t,x) = n\left(c - \frac{1}{(1+n)\,(1+c)}\right), & t \geq 0, \ x \in \mathbb{R}^2, \\ \frac{\partial}{\partial t} c(t,x) - d_2 \Delta c(t,x) = -nc, \\ \frac{\partial}{\partial t} f(t,x) = n\, \frac{1}{(1+n)\,(1+c)}. \end{cases} \tag{5.12}$$

Here $n(t,x)$ represents active cells: they consume nutrients, move, multiply and can change to the state f of ‘frozen’ cells (that do not move, do not consume nutrients, do not multiply and never change state). The concentration of nutrients is denoted

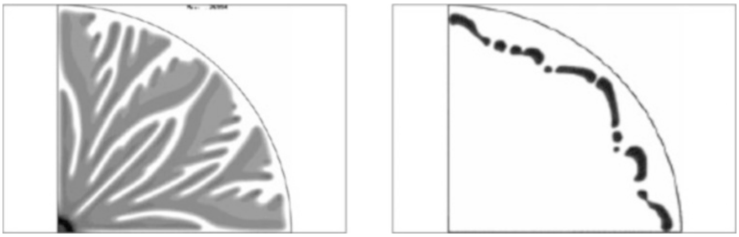

Fig. 5.11 Solutions given by the Mimura system (5.12) with a higher nutrients level c than in Fig. 5.10. Computations by A. Marrocco

by c; it diffuses according to molecular diffusion rules and is consumed by active cells.

The initial data represents an *inoculum*, i.e., a small amount of bacteria located at the center of the ball (the computational domain). The reason why the dentritic dynamic pattern occurs in this model is very close to that in the Gray-Scott system. The solution cell population density $n(t,x)$ to the first equation has a tendency to create Dirac concentrations. These concentrations move towards the larger values of the nutrients c, and this is the boundary of the computational domain. Indeed, nutrients are consumed progressively inside the domain and this creates a nutrient gradient towards the boundary.

One can explain intuitively this ‘nutrient instability’. Cells which are a little in front of the others find higher concentrations of nutrients. Therefore, they multiply faster and by diffusion generate new cells which advance even more at the front. Around these cells the nutrients are depleted and this leads to a slow-down of multiplication, creating a branch that goes forward.

5.3.3 Branching Instabilities

However, the ‘nutrient instability’ is likely insufficient to explain the complex phenomena of swarming (a massive coordinated migration, see Fig. 5.8) in particular on a medium rich in nutrients.

Biophysical factors can also lead to branching instabilities, which do not depend on the mechanism of ‘nutrient instability’ but only on various forces (compatible with effects of surface tension) acting on the colony. This is the case of surfactants, which are certainly involved in the phenomena. To represent forces, lead us to write a nonlinear Fokker-Planck equation (see Chap. 8). For this material, we only refer to B. Perthame et al. [24]. Figure 5.12 shows snapshots of the branching patterns arising in this nonlinear Fokker-Planck equation.

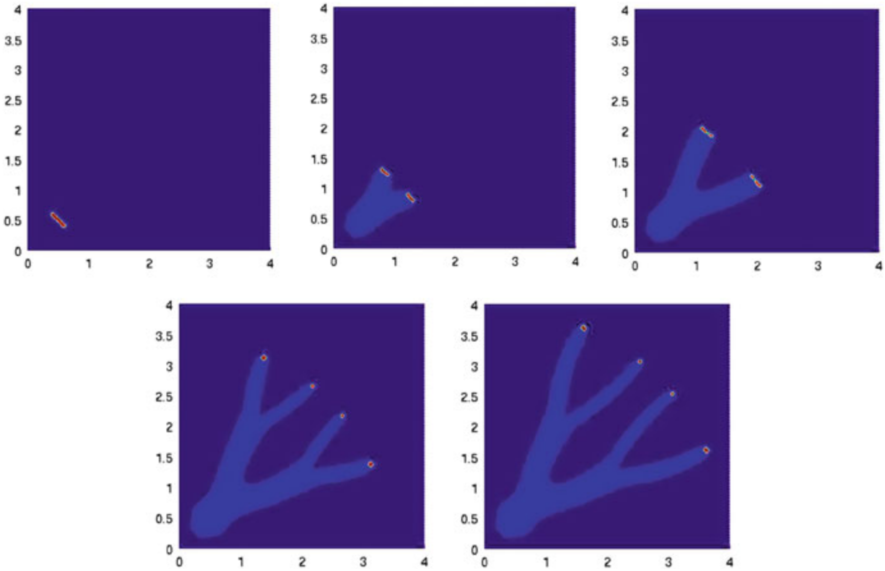

Fig. 5.12 Snapshots of the branching pattern as they arise in the nonlinear Fokker-Planck equation as explained in Sect. 5.3.3. Reproduced using a software by N. Vauchelet and based on a model analyzed in F. Cerreti, B. Perthame, C. Schmeiser, M. Tang and N. Vauchelet, Waves for a hyperbolic Keller-Segel model and branching instabilities. M3AS 21 suppl. (2011) 825–842

5.3.4 Spiral Waves

Spiral waves are observed in various fields of science. Two typical examples are the Belousov-Zabotinsky chemical reaction and heart electrophysiology, see [17] and M. Thiriet [27]. In medicine, these spiral waves are commonly observed and are known to be responsible for pathologies such as *heart fibrillation*. They are also observed on the retina and in the cerebral cortex where they are supposedly related to epilepsy [28].

In parabolic systems, theoretical explanations of the generation of spiral waves are available [1]. Parabolic systems such as the FitzHugh-Nagumo in two dimensions are able to produce this type of solution with a range of parameters, where the constant steady state is Turing unstable (see Sect. 7.5.7). We use the system written as (here c is a positive constant)

$$\begin{cases} \tau \frac{\partial}{\partial t} u(t,x) - d\Delta u(t,x) = u - \frac{u^3}{3} - v, \qquad t \geq 0,\ x \in [0,1]^2, \\ \qquad\qquad\qquad\quad \frac{\partial}{\partial t} v(t,x) = -u - c - \gamma v. \end{cases} \tag{5.13}$$

Numerical solutions are obtained with initial data composed of four values in the four quadrants of the computational domain (a square). These are again dynamic patterns and Fig. 5.13 shows the solution at three different times.

Fig. 5.13 Snapshots of the *spiral wave* solution of the FitzHugh- Nagumo system (5.13) at three different times for parameters $\tau = 0.01$, $c = 0.2$, $d = 10^{-5}$, $\gamma = 0.5$. Based on a FreeFEM++ code [13, 15] by Y. Deleuze

H. Murakawa and H. Ninomiya [20] have observed recently that spiral waves can also occur in three species competition systems with an appropriate choice of parameters. They relate this phenomena to the segregation property, see Sect. 8.11. The system they use is

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - d_u \Delta u(t,x) = ku\big(1 - u - \alpha v - \beta w\big), \\ \frac{\partial}{\partial t}v(t,x) - d_v \Delta v(t,x) = kv\big(1 - \beta u - v - \alpha w\big), \\ \frac{\partial}{\partial t}w(t,x) - d_w \Delta w(t,x) = kw\big(1 - \alpha u - \beta v - w\big). \end{cases}$$

Here, the segregation property means that, as $k \to \infty$ only one component u, v or w is positive the other two components vanish. See also Chap. 10 and S.-I. Ei et al. [11].

References

1. Alford, J.G., Auchmuty, G.: Rotating wave solutions of the FitzHugh-Nagumo equations. J. Math. Biol. **53**(5), 797–819 (2006)
2. Aliev, R., Panfilov, A.: A simple two-variable model of cardiac excitation. Chaos Solitons Fractals **3**(7), 293–301 (1996)
3. Baker, R.E., Gaffney, E.A., Maini, P.K.: Partial differential equations for self-organization in cellular and developmental biology. Nonlinearity **21**, R251–R290 (2008)
4. Barles, G.: Solutions de viscosité des équations de Hamilton-Jacobi. Springer, Berlin/Heidelberg (1994)
5. Ben Amar, M., Chatelain, C., Ciarletta, P.: Contour instabilities in early tumor growth models. PRL **106**, 148101 (2011)
6. Blanchet, A., Dolbeault, J., Perthame, B.: Two-dimensional Keller-Segel model: optimal critical mass and qualitative properties of the solutions. Electron. J. Diff. Equ. **2006**(44), 1–32 (2006)
7. Calvez, V., Carrillo, J.A.: Volume effects in the Keller-Segel model: energy estimates preventing blow-up. J. Math. Pures et Appl. **86**(2), 155–175 (2006)

8. Chalub, F., Rodriguez, J.-F.: Proceedings of the Conference ‘The Mathematics of Darwin’s Legacy’, Lisbon, 2010. Birkhauser (Basel) Series Mathematics and Biosciences in Interaction (2011)
9. Ciarletta, P., Foret, L., Ben Amar, M.: The radial growth phase of malignant melanoma: multi-phase modeling, numerical simulations and linear stability analysis. J. R. Soc. Interface **8**(56), 345–368 (2011)
10. Diekmann, O.: A beginner’s guide to adaptive dynamic. In: Rudnicki, R. (ed.) Mathematical Modeling of Population Dynamic. Banach Center Publications, vol. 63, pp. 47–86. Polish Academy of Sciences, Warsaw (2004)
11. Ei, S.-I., Ikota, R., Mimura, M.: Segregating partition problem in competition-diffusion systems. Interfaces Free Bound **1**, 57–80 (1999)
12. Françoise, J.-P.: Oscillations en biologie. Collection Mathématiques et Applications. SMAI, Springer, Paris (2005)
13. FreeFEM++: Software available at http://www.freefem.org (2015)
14. Golding, I., Kozlovski, Y., Cohen, I., BenJacob, E.: Studies of bacterial branching growth using reaction-diffusion models for colonial development. Physica A **260**, 510–554 (1998)
15. Hecht, F.: New development in FreeFEM++. J. Numer. Math. **20**(3–4), 251–265 (2012)
16. Hillen, T., Painter, K.: A user’s guide to PDE models for chemotaxis. J. Math. Biol. **58**(1), 183–217 (2009)
17. Keener, J., Sneyd, J.: Mathematical Physiology. Springer, New York (2008)
18. Kolokolnikov, T., Ward, M.J., Wei, J.: The existence and stability of spike equilibria in the one-dimensional Gray-Scott model: the pulse-splitting regime. Physica D **202**, 258–293 (2005)
19. Mimura, M., Sakaguchi, H., Matsuchita, M.: Reaction diffusion modeling of bacterial colony patterns. Physica A **282**, 283–303 (2000)
20. Murakawa, H., Ninomiya, H.: Fast reaction limit of a three-component reaction-diffusion system. J. Math. Anal. Appl. **379**(1), 150–170 (2011)
21. Muratov, C., Ospinov, V.V.: Stability of the static spike autosolitons in the Gray-Scott model. SIAM J. Appl. Math. **62**(5), 1463–1487 (2002)
22. Murray, J.D.: Mathematical Biology, vols. 1 and 2, 2nd edn. Springer, New York (2002)
23. Perthame, B.: Transport Equations Arising in Biology. L. N. series ‘Frontiers in Mathematics’. Birkhauser, Basel (2007)
24. Perthame, B., Schmeiser, C., Tang, M., Vauchelet, N.: Traveling plateaus for a hyperbolic Keller-Segel system with attraction and repulsion: existence and branching instabilities. Nonlinearity **24**, 1253–1270 (2011)
25. Roger, J.M., McCulloch, A.D.: A collocation-Galerkin finite element model of cardiac action potential propagation. IEEE Trans. Biomed. Eng. **41**, 743–757 (1994)
26. Stevens, A.: Derivation of chemotaxis-equations as limit dynamic of moderately interacting stochastic many particle systems. SIAM J. Appl. Math. **61**, 183–212 (2000)
27. Thiriet, M.: Tissue Functioning and Remodeling in the Circulatory and Ventilatory Systems. Springer, Berlin (2013)
28. Winfree, A.: Are cardiac waves relevant to epileptic wave propagation? In: Milton, J., Jung, P. (eds.) Epilepsy as a Dynamical Disease, Chap. 10. Springer, Berlin (2003)

Chapter 6
Blow-Up and Extinction of Solutions

We know from Chap. 2 that for 'small' nonlinearities, the solutions of parabolic systems relax to an elementary state. When the nonlinearity is too large, it is possible that solutions of nonlinear parabolic equations do not exist for all times or simply vanish, two scenarios that are the first signs of visible nonlinear effects.

The mechanisms can be seen in simple ordinary differential equations. *Blow-up* means that the solution becomes pointwise larger and larger and eventually becomes infinite in finite time. To see this, consider the equation

$$\dot{z}(t) = z(t)^q, \qquad z(0) > 0, \qquad q > 1.$$

Its solution $z(t) > 0$ is given by

$$z(t)^{q-1} = z(0)^{q-1} / \big(1 - (q-1)tz(0)^{q-1}\big)$$

and thus it tends to infinity at $t = T^* := \frac{1}{(q-1)z(0)^{q-1}}$. For $q = 2$, it is a typical illustration of the alternative arising in the Cauchy-Lipschitz Theorem; solutions can only tend to infinity in finite time (case $z(0) > 0$), or they are globally defined (case $z(0) < 0$).

The mechanism of extinction is illustrated by the equation with the opposite sign

$$\dot{z}(t) = -z(t)^q, \qquad z(0) > 0, \qquad q > 1.$$

Its solution

$$z(t)^{q-1} = z(0)^{q-1} / \big(1 + (q-1)tz(0)^{q-1}\big) \tag{6.1}$$

vanishes as $t \to \infty$.

The purpose of this chapter is to study in which respect these phenomena can occur or not when diffusion is added.

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_6

We begin with the semilinear parabolic equation with Dirichlet boundary conditions

$$\frac{\partial}{\partial t}u - \Delta u = u^2.$$

We present several methods for proving blow-up in finite time. The first two methods are for semi-linear parabolic equations, the third method is illustrated by the Keller-Segel system for chemotaxis; this is more interesting because it blows-up in all L^p norms, for all $p > 1$, but the L^1 norm is conserved (this represents the total number of cells in a system where cell multiplication is ignored).

The last section is devoted to a counter-intuitive result with respect to extinction.

6.1 Semilinear Equations: The Method of the Eigenfunction

To study the case of nonlinear parabolic equations, we consider the model

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = u^2, & t \geq 0,\ x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \\ u(t=0,x) = u^0(x) \geq 0. \end{cases} \tag{6.2}$$

Here we treat the case when Ω is a bounded domain. To define a distributional solution is not completely obvious because the right hand side u^2 should be well defined, that is why we require that u belongs to L^2; then it remains to solve the heat equation with a right hand side in L^1. That is why we call *solution of* (6.2), a function satisfying for some $T > 0$,

$$u \in L^2\big((0,T)\times\Omega\big), \qquad u \in C\big([0,T);L^1(\Omega)\big). \tag{6.3}$$

The question then is to know if effects of diffusion are able to overcome the effects of quadratic nonlinearity and (6.2) could have global solutions. The answer is given by the next theorems

Theorem 6.1 *Assume that Ω is a bounded domain, $u^0 \geq 0$, u^0 is sufficiently large (in a weighted L^1 space introduced below), then there is a time T^* for which the solution of* (6.2) *satisfies*

$$\|u\|_{L^2([0,T)\times\mathbb{R}^d)} \underset{T\to T^*}{\longrightarrow} \infty.$$

Of course, this result means that $u(t)$ also blows up in all L^p norms, $2 \le p \le \infty$ because we work in a bounded domain. It is also possible to prove that the blow-up time is the same for all these norms [6].

Proof of Theorem 6.1 We are going to arrive at a contradiction in the hypothesis that a function $u \in L^2\big((0,T) \times \Omega\big)$ can be a solution of (6.2) when T exceeds an explicit value computed later.

First we, notice that $u(t,x) \ge 0$ because $u^0 \ge 0$.

Because we are working in a bounded domain, the smallest eigenvalue of the operator $-\Delta$ exists and is associated with a positive eigenfunction (see Sect. 2.5)

$$\begin{cases} -\Delta w_1 = \lambda_1 w_1, \qquad w_1 > 0 \qquad \text{in } \Omega, \\ w_1(x) = 0, \; x \in \partial\Omega, \qquad \int_\Omega (w_1)^2 = 1. \end{cases} \tag{6.4}$$

For a solution, we can multiply Eq. (6.2) by w_1 and integrate by parts. We arrive at

$$\begin{aligned} \frac{d}{dt}\int_\Omega u(t,x)\, w_1(x)\, dx &= \int_\Omega \Delta u(t,x)\, w_1(x)\, dx + \int_\Omega u(t,x)^2\, w_1(x)\, dx \\ &= \int_\Omega u(t,x)\, \Delta w_1(x)\, dx + \int_\Omega u(t,x)^2\, w_1(x)\, dx \\ &= -\lambda_1 \int_\Omega u(t,x)\, w_1(x)\, dx + \int_\Omega u(t,x)^2\, w_1(x)\, dx \\ &\ge -\lambda_1 \int_\Omega u(t,x)\, w_1(x)\, dx \\ &\quad + \left(\int_\Omega u(t,x)\, w_1(x)\, dx\right)^2 \left(\int_\Omega w_1(x)\, dx\right)^{-1} \end{aligned}$$

(after using the Cauchy-Schwarz inequality). We set $z(t) = e^{\lambda_1 t} \int_\Omega u(t,x) \;\; w_1(x)$ and, with $a = \big(\int_\Omega w_1(x)\, dx\big)^{-1}$, the above inequality reads

$$\frac{d}{dt} z(t) \ge a e^{-\lambda_1 t}\, z(t)^2,$$

and we obtain:

$$\frac{d}{dt}\frac{1}{z(t)} \le -a e^{-\lambda_1 t},$$

$$\frac{1}{z(t)} \le \frac{1}{z^0} - a\frac{1 - e^{-\lambda_1 t}}{\lambda_1}.$$

Assume now the size condition

$$z^0 > \frac{\lambda_1}{a}. \tag{6.5}$$

The above inequality contradicts that $z(t) > 0$ for $e^{-\lambda_1 t} \leq 1 - \frac{\lambda_1}{az^0}$. Therefore, the computation, and thus the assumption that $u \in L^2((0,T) \times \mathbb{R}^d)$, fails before that finite time. □

The size condition is necessary. There are various ways to understand this. For $d \leq 5$ it follows from a general elliptic equation

Theorem 6.2 *There is a steady state solution $\bar{u} > 0$ in Ω to*

$$\begin{cases} -\Delta u = u^p, & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \end{cases}$$

when p satisfies

$$1 < p < \frac{d+2}{d-2}.$$

We refer to [2] for a proof of this theorem and related results (as non-existence for $p > \frac{d+2}{d-2}$).

One can see more directly that the size condition is needed. We choose $\mu = \min_\Omega \frac{\lambda_1}{w_1(x)}$ and set $\tilde{w} = \mu w_1$. This is a supersolution of (6.2) because

$$\frac{\partial}{\partial t}\tilde{w} - \Delta\tilde{w} = \lambda_1 \tilde{w} \geq \tilde{w}^2.$$

One concludes that, when $u^0 \leq \tilde{w}$, solutions of (6.2) satisfy $u(t) \leq \tilde{w}$ for all times t, as long as the solution exists (and this is sufficient to prove that the solution is global). Therefore, we have the

Lemma 6.3 *Under the smallness condition $u^0 \leq \min_\Omega \frac{\lambda_1}{w_1(\cdot)} w_1$, there is a global solution of (6.2) and $u(t) \leq \tilde{w}$, $\forall t \geq 0$.*

Proof We subtract a solution u to $\tilde{w}$ and find

$$\frac{\partial}{\partial t}[u - \tilde{w}] - \Delta[u - \tilde{w}] \leq u^2 - \tilde{w}^2 = [u - \tilde{w}][u + \tilde{w}],$$

with $u - \tilde{w}(t = 0) \leq 0$. From the comparison principle, we conclude that $u - \tilde{w}(t) \leq 0$ for all times where the solution exists. Therefore, by continuation methods, there is a global solution. □

Exercise Prove blow-up in finite time for the case of a general nonlinearity

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = f(u), & t \geq 0, \ x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \\ u(t=0,x) = u^0(x) > 0 & \text{large enough}, \end{cases} \tag{6.6}$$

and $f(u) \geq cu^\alpha$ with $\alpha > 1$.

Exercise (Neumann Boundary Conditions) A solution in $[0, T)$ of the equation

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = u^2, & t \geq 0, \ x \in \Omega, \\ \frac{\partial}{\partial \nu}u(x) = 0, \ x \in \partial\Omega, \\ u(t=0,x) = u^0(x) > 0, \end{cases} \tag{6.7}$$

is a distributional solution satisfying $u \in L^2([0,T) \times \Omega)$.

1. Prove that there is no such solution after some time T^* and no size condition is required here.
2. Prove also that $\|u(T)\|_{L^1(\mathbb{R}^d)} \xrightarrow[T \to T^*]{} \infty$.

Exercise For $d = 1$ and $\Omega =]-1,1[$, construct a unique, even and non-zero solution of

$$-\Delta v = v^2, \qquad v(\pm 1) = 0.$$

Hint. Reduce it to $-\frac{1}{2}(v')^2 = \frac{1}{3}v^3 + c_0$ and find a positive real number c_1 such that

$$v' = -\sqrt{c_1 - \frac{2}{3}u^3}.$$

6.2 Semilinear Equations: The Energy Method

Still considering semilinear parabolic equations, we present another method leading to a different size condition. This better uses the intrinsic properties of the equation and does not use the sign condition.

We consider a more general case with $p > 1$

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = |u|^{p-1}u, & t \geq 0, \ x \in \Omega, \\ u(x) = 0, \ x \in \partial\Omega, \\ u(t=0,x) = u^0(x) \neq 0. \end{cases} \tag{6.8}$$

Before we state our result, it is useful to recall the energy principle underlying this equation. We define the energy

$$E(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 - \frac{1}{p+1}\int_\Omega |u|^{p+1}.$$

Note that this has a mechanical interpretation: the term $\frac{1}{2}\int_\Omega |\nabla u|^2$ is the kinetic energy and the term $-\frac{1}{p+1}\int_\Omega |u|^{p+1}$ is the potential energy.

One can easily see that this energy decreases with time (in fact this comes from the structure of a *gradient flow* for (6.8)). Indeed, using the chain rule and integration by parts, we have

$$\begin{aligned}\tfrac{d}{dt}E\big(u(t)\big) &= \quad \textstyle\int_\Omega \big[\nabla u.\nabla \frac{\partial u}{\partial t} - |u|^{p-1}u\frac{\partial u}{\partial t}\big] \\ &= -\textstyle\int_\Omega \frac{\partial u}{\partial t}\big[\Delta u + |u|^{p-1}u\big] \\ &= -\textstyle\int_\Omega \big[\Delta u + |u|^{p-1}u\big]^2 \le 0.\end{aligned}$$

Consequently, we have

$$E(t) \le E^0 := E(u^0). \tag{6.9}$$

This explains the central role of the energy in the

Theorem 6.4 *For $u^0 \in H_0^1(\Omega)$ satisfying $E(u^0) \le 0$, there are no global solution of* (6.8) *with bounded energy.*

Proof We define $\alpha = \frac{1}{2} - \frac{1}{p+1} > 0$. We combine the L^2-estimate with the energy decay and obtain

$$\begin{aligned}\tfrac{1}{4}\tfrac{d}{dt}\textstyle\int_\Omega u^2 dx &= -\tfrac{1}{2}\textstyle\int_\Omega[\,|\nabla u|^2 - |u|^{p+1}]dx \\ &= -E(u) + \alpha \textstyle\int_\Omega |u|^{p+1} \\ &\ge -E(u^0) + \alpha|\Omega|^{(1-p)/2}\big(\textstyle\int_\Omega u^2\big)^{(p+1)/2}.\end{aligned}$$

The last inequality uses Jensen's inequality for the probability measure $dx/|\Omega|$

$$\left(\int_\Omega u^2 \frac{dx}{|\Omega|}\right)^{(p+1)/2} \le \int_\Omega u^{p+1}\frac{dx}{|\Omega|}.$$

This proves blow-up for $E(u^0) \le 0$ because the positive function $z(t) := \int_\Omega u^2$ satisfies

$$\frac{dz(t)}{dt} \ge \beta z(t)^{(p+1)/2}, \qquad \beta := \alpha|\Omega|^{(1-p)/2} > 0,$$

and thus it blows-up in finite time, as shown in the introduction. $\square$

Exercise Find functions $u^0 \in H_0^1(\Omega)$ that satisfy the condition $E(u^0) \le 0$.

Hint. Use the fact that the two terms in the definition of the energy have different scales in u and consider expressions as $rV(x)$.

Exercise Prove blow-up for $\left(\int_\Omega (u^0)^2\right)^{(p+1)/2} > \frac{2}{\beta} E(u^0)$.

The topic of blow-up is very rich and many modalities of blow-up, different blow-up rates, blow-up for different norms and regularizing effects that prevent blow-up are also possible. See [6].

6.3 Keller-Segel System: The Method of Moments

We come back to the Keller-Segel model used to describe chemotaxis as mentioned in Sect. 8.9. We recall that it consists of a system which describes the evolution of the population density of cells (bacteria, amoeba, ...) $n(t,x)$, $t \ge 0$, $x \in \mathbb{R}^d$ and the concentration $c(t,x)$ of the attracting molecules released by the cells themselves,

$$\begin{cases} \frac{\partial}{\partial t} n - \Delta n + \operatorname{div}(n\chi \nabla c) = 0, \qquad t \ge 0,\ x \in \mathbb{R}^d, \\ -\Delta c + \tau\, c = n, \\ n(t=0) = n^0 \in L^\infty \cap L^1_+(\mathbb{R}^d). \end{cases} \tag{6.10}$$

The first equation expresses the random (Brownian) diffusion of the cells with a bias directed by the chemoattractant concentration with a sensitivity χ. The case $\chi = 0$ means the cells do not react. The chemoattractant c is directly released by the cell, diffuses on the substrate and is degraded with a coefficient τ that scales in a such a way that $\tau^{-1/2}$ represents the *activation length*.

The notation L^1_+ means nonnegative integrable functions, and the parabolic equation for n gives nonnegative solutions (as expected for the cell density, see Chap. 8)

$$n(t,x) \ge 0, \qquad c(t,x) \ge 0. \tag{6.11}$$

Another property we use is the conservation of the total number of cells

$$m^0 := \int_{\mathbb{R}^d} n^0(x)\, dx = \int_{\mathbb{R}^d} n(t,x)\, dx. \tag{6.12}$$

In particular, solutions cannot blow-up in L^1. But we have the

Theorem 6.5 *In $\mathbb{R}^2$, take $\tau = 0$ and assume $\int_{\mathbb{R}^2} |x|^2 n^0(x)dx < \infty$.*

(i) (Blow-up) When the initial mass satisfies

$$m^0 := \int_{\mathbb{R}^2} n^0(x)dx > m_{\text{crit}} := 8\pi/\chi, \tag{6.13}$$

then any solution of (6.10) *becomes a singular measure in finite time.*

(ii) When the initial data satisfies $\int_{\mathbb{R}^2} n^0(x)|\log(n^0(x))|dx < \infty$ and

$$m^0 := \int_{\mathbb{R}^2} n^0(x)dx < m_{\text{crit}} := 8\pi/\chi, \tag{6.14}$$

there are weak solutions of (6.10) *satisfying the* a priori *estimates*

$$\int_{\mathbb{R}^2} n[|\ln(n(t))| + |x|^2]\, dx \le C(t),$$

$$\|n(t)\|_{L^p(\mathbb{R}^2)} \le C(p,t,n^0) \qquad \textit{for} \;\; \|n^0\|_{L^p(\mathbb{R}^2)} < \infty, \quad 1 < p < \infty.$$

Here we only explain the argument for blow-up. We refer to [1, 5] for the complete proof of Theorem 6.5.

Proof We follow Nagai's [4] argument based on the method of moments, assuming sufficient decay in x at infinity. This is based on the formula

$$\nabla c(t,x) = -\lambda_2 \int_{\mathbb{R}^2} \frac{x-y}{|x-y|^2} n(t,y)dy, \qquad \lambda_2 = \frac{1}{2\pi}.$$

Then, we consider the second x moment

$$m_2(t) := \int_{\mathbb{R}^2} \frac{|x|^2}{2} n(t,x)dx.$$

We have, from (6.10),

$$\begin{aligned}
\tfrac{d}{dt} m_2(t) &= \textstyle\int_{\mathbb{R}^2} \frac{|x|^2}{2} [\Delta n - \operatorname{div}(n\chi\nabla c)]dx \\
&= \textstyle\int_{\mathbb{R}^2} [2n + \chi n x\cdot \nabla c]dx \\
&= 2m^0 - \chi\lambda_2 \textstyle\int_{\mathbb{R}^2\times\mathbb{R}^2} n(t,x)n(t,y)\frac{x\cdot(x-y)}{|x-y|^2} \\
&= 2m^0 - \frac{\chi\lambda_2}{2} \textstyle\int_{\mathbb{R}^2\times\mathbb{R}^2} n(t,x)n(t,y)\frac{(x-y)\cdot(x-y)}{|x-y|^2}
\end{aligned}$$

(this last equality simply follows by a symmetry argument, interchanging x and y in the integral). This yields finally,

$$\frac{d}{dt}m_2(t) = 2m^0(1 - \frac{\chi}{8\pi}m^0).$$

Therefore, if we have $m^0 > 8\pi/\chi$, we arrive at the conclusion that $m_2(t)$ should become negative in finite time, which is impossible since n is nonnegative. Consequently, the solution cannot be smooth until that time. □

6.4 Non-extinction

We consider now a nonlinearity with the negative sign, still with $p > 1$,

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = -u^p, & t \geq 0,\ x \in \mathbb{R}^d, \\ u(t=0,x) = u^0(x) > 0. \end{cases} \tag{6.15}$$

We recall that the solution remains positive $u(t,x) > 0$.

As pointed out in the introduction, in the absence of diffusion, the solution (6.1) vanishes in infinite time. Does diffusion change this effect?

To analyze this issue, we define the total mass

$$M(t) = \int_{\mathbb{R}^d} u(t,x)dx$$

which clearly decreases

$$\frac{d}{dt}M(t) = -\int_{\mathbb{R}^d} u^p(t,x)dx < 0. \tag{6.16}$$

Following [3], we are going to prove *non-extinction* when diffusion is present

Theorem 6.6 *Assume $p > 1 + \frac{2}{d}$ and $u^0 \in L^1 \cap L^\infty(\mathbb{R}^d)$, then the solution of* (6.17) *satisfies*

$$\lim_{t\to\infty} M(t) > 0.$$

There is a nice biological interpretation in [3] related to the phenomena of so-called *broadcast-spawning*. This is an external fertilization strategy used by various benthic invertebrates (sea urchins, anemones, corals, jellyfish) whereby males and females release at the same time, short lived sperm and egg gametes into the surrounding flow. The gametes are positively buoyant, and rise to the surface of the ocean. The fertilized gametes form larva and are negatively buoyant and sink to the bottom of the ocean floor to start a new colony. For the coral spawning problem, field measurements of the fertilization rates are often as high as 90 %. To arrive at such high rates, rapid dispersion on the ocean surface is required for successful encounters and, as shown above, diffusion is clearly not sufficient, additional chemotactic attraction is certainly involved.

The model at hand supposes that sperm and eggs have the same density (but this assumption can be released in a system of two parabolic equations, arriving at the same conclusion, see below). Chemotaxis is omitted. The parameter $p = 2$ represents binary interactions leading to fertilized eggs that are withdrawn from the balance equation. The theorem shows that, in the absence of chemotaxis, not all the eggs are fertilized. In [3] it is proved that chemoattraction increases this rate but additional flow mixing does not.

Proof Our assumption for p is equivalent to $\delta = (p-1)d/2 - 1 > 0$.

First Step. A Lower Bound For all $t > \tau > 0$, we can estimate, thanks to (3.24) with initial time τ,

$$\int_{\mathbb{R}^d} u^p(t,x)dx \le C(d,p)\; M(\tau)^p \;(t-\tau)^{-1-\delta}.$$

Therefore, we can write for $T \ge \tau + a$, and $a > 0$,

$$\begin{aligned} M(T) &= M(\tau+a) - \int_{\tau+a}^{T}\int_{\mathbb{R}^d} u^p(t,x)dxdt \\ &\ge M(\tau+a) - C(d,p)M(\tau)^p \int_{\tau+a}^{T} (t-\tau)^{-1-\delta}dt, \end{aligned}$$

and thus,

$$M(T) \ge M(\tau+a) - C(d,p)M(\tau)^p\; a^{-\delta}.$$

Second Step. A Upper Bound Let $\tilde{u}$ be the solution to the linear equation

$$\begin{cases} \frac{\partial}{\partial t}\tilde{u} - \Delta\tilde{u} = 0, & t \ge 0,\; x \in \mathbb{R}^d, \\ \tilde{u}(t=0,x) = u^0(x) > 0. \end{cases} \tag{6.17}$$

We have $u \le \tilde{u}$ and thus, thanks to (3.24),

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \le C(d,p)M(0)^p\; t^{-1-\delta}.$$

Therefore, we find

$$M(\tau+a) \ge M(\tau) - \int_{\tau}^{\tau+a}\int_{\mathbb{R}^d} u^p(t,x)dxdt.$$

Because $M(\cdot)$ is non-increasing, we finally obtain

$$M(\tau + a) \geq M(\tau) - a\|u^0\|^{p-1}_{L^\infty(\mathbb{R}^d)} M(\tau).$$

Third Step. Conclusion Combining these two steps, and choosing a with the rule $a\|u^0\|^{p-1}_{L^\infty(\mathbb{R}^d)} = 1/2$, we obtain

$$M(T) \geq \frac{1}{2} M(\tau) - C(d,p) M(\tau)^p \, a^{-\delta}.$$

If we had $M(T) \to 0$ as $T \to \infty$, we would conclude that

$$C(d,p) M(\tau)^{p-1} \, a^{-\delta} \geq \frac{1}{2},$$

which contradicts that $M(\tau)$ can vanish for large values of τ.

This proves the result. $\square$

Exercise From the above argument derive an explicit bound for the minimum mass (depending on $M(0)$, p, d).

Exercise Assume $u^0 \in L^1 \cap L^\infty(\mathbb{R}^d)$ and consider the equation without diffusion

$$\frac{\partial}{\partial t} u = -u^p, \qquad t \geq 0, \; x \in \mathbb{R}^d.$$

Show that $\int_{\mathbb{R}^d} u(t,x)dx \to 0$ as $t \to \infty$.

Exercise Consider the system for eggs and other gametes (sperm)

$$\begin{cases} \frac{\partial}{\partial t} e - d_e \Delta e = -(eg)^{p/2}, & t \geq 0, \; x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} g - d_g \Delta g = -(eg)^{p/2}, & \\ e(t=0,x) = e^0(x) > 0. & g(t=0,x) = g^0(x) > 0 \end{cases}$$

Show that both $\lim_{t\to\infty} \int_{\mathbb{R}^d} e(t,x)dx$ and $\lim_{t\to\infty} \int_{\mathbb{R}^d} g(t,x)dx$ are positive.

See [3] again.

References

1. Blanchet, A., Dolbeault, J., Perthame, B.: Two-dimensional Keller-Segel model: optimal critical mass and qualitative properties of the solutions. Electron. J. Diff. Equ. **2006**(44), 1–32 (2006)
2. Evans, L.C.: Partial Differential Equations. Graduate Studies in Mathematics, vol. 19. American Mathematical Society, Providence, RI (1998)

3. Kiselev, A., Ryzhik, L.: Biomixing by chemotaxis and enhancement of biological reactions. Commun. Partial Diff. Equ. **37**, 298–318 (2012)
4. Nagai, T.: Blow-up radially symmetric solutions to a chemotaxis system. Adv. Math. Appl. Sci. **5**, 581–601 (1995)
5. Perthame, B.: Transport Equations Arising in Biology. L. N. Series 'Frontiers in Mathematics'. Birkhauser, Basel (2007)
6. Quittner, P., Souplet, P.: Superlinear Parabolic Problems. Blow-Up, Global Existence and Steady State. Birkhäuser Advanced Texts. Birkhäuser, Basel (2007)

Chapter 7
Linear Instability, Turing Instability and Pattern Formation

In his seminal paper [33] A. Turing "suggests that a system of chemical substances reacting together and diffusing through a tissue, is adequate to account for the main phenomena of morphogenesis". He introduces several concepts associated with the chemical basis of morphogenesis (and the name 'morphogen' itself), spatial chemical patterns, and what is now called 'Diffusion Driven Instability'. The concept of *Turing instability* has become standard and the aim of this chapter is to describe what it is (and what it is not!).

The first numerical simulations of a system exhibiting Turing patterns was published in 1972 involving the celebrated system of Gierer and Meinhardt [9] (see also Sect. 7.5.8).

It was only 20 years later that the first experimental evidence for a chemical reaction exhibiting spatial patterns explained by these principles was obtained. This reaction is named the *CIMA reaction* after the name of the reactants used by P. De Kepper et al. [6] and Castets et al. [5]. See also Sect. 7.5.2.

In 1995, S. Kondo and R. Asai [14] found an explanation of the patterns arising during the development of animals, proposing that the model should be set in a growing domain, thus opening up a larger class of possible patterns. Spots, which are a usual steady state for Turing systems in a fixed domain, can more easily give way to bands in a growing domain.

Meanwhile, several nonlinear parabolic systems exhibiting Turing Patterns have been studied. Some have been aimed at modeling particular examples of morphogenesis such as the models developed in [21, 22]. Some have been derived as the simplest possible models exhibiting Turing instability conditions. Nowadays, the biological interest in morphogenesis has evolved towards molecular cascades, pathways and genetic networks. Some biologists doubt that, within cells or tissues, diffusion provides an adequate description of molecular spreading. However, Turing's mechanism remains both the simplest explanation for pattern formation, and one of the most counter-intuitive results in the field of Partial Differential Equations.

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_7

This chapter presents Turing's theory and several examples of diffusion driven instabilities. We begin with the historical example of reaction-diffusion systems where the linear theory shows its exceptional originality. Then we present nonlinear examples. The simplest of the latter is the non-local Fisher/KPP equation, while some more standard parabolic systems are also presented.

7.1 Turing Instability in Linear Reaction-Diffusion Systems

An amazingly counter-intuitive observation is the instability mechanism proposed by A. Turing [33]. Consider a linear 2×2 O.D.E. system

$$\begin{cases} \frac{du}{dt} = au + bv, \\ \frac{dv}{dt} = cu + dv, \end{cases} \tag{7.1}$$

with real constant coefficients a, b, c and d. We assume that

$$\mathcal{T} := a + d < 0, \qquad \mathcal{D} := ad - bc > 0. \tag{7.2}$$

Consequently, we have

$$(u, v) = (0, 0) \text{ is a stable attractive point for the system (7.1).} \tag{7.3}$$

In other words, the matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

has two eigenvalues with negative real parts (or a single negative eigenvalue and a Jordan form). Indeed, its characteristic polynomial is

$$(a - X)(d - X) - bc = X^2 - X\mathcal{T} + \mathcal{D},$$

and the two complex roots are $X_\pm = \frac{1}{2}[\mathcal{T} \pm \sqrt{\mathcal{T}^2 - 4\mathcal{D}}]$.

Now consider a bounded domain Ω of $\mathbb{R}^d$ and add diffusion to the system (7.1),

$$\begin{cases} \frac{\partial u}{\partial t} - \sigma_u \Delta u = au + bv, \qquad x \in \Omega, \\ \frac{\partial v}{\partial t} - \sigma_v \Delta v = cu + dv, \end{cases} \tag{7.4}$$

with either a Neumann or a Dirichlet boundary condition. In both cases, the state $(u, v) = (0, 0)$ is still a steady solution, of (7.4).

In principle, adding diffusion to the differential system (7.1) should increase stability. But surprisingly we have

Theorem 7.1 (Turing Instability Theorem) *Consider the system* (7.4) *where we fix the domain* Ω *and the matrix* A *and* $\sigma_v > 0$. *We assume* (7.2) *with* $a > 0$, $d < 0$. *Then, for* σ_u *sufficiently small, the steady state* $(u, v) = (0, 0)$ *is linearly unstable. Moreover, only a finite number of eigenmodes are unstable.*

The usual interpretation of this result is as follows. Because $a > 0$ and $d < 0$, the quantity u is called an activator and v an inhibitor. On the other hand, fixing a unit of time, the σ's are scaled as the square of length. The result can be extended as the

Turing Instability Alternative

- Turing instability $\iff$ short range activator, long range inhibitor.
- Traveling waves $\iff$ long range activator, short range inhibitor.

There is no general proof of this statement, which can only be applied to nonlinear systems. But it is a general observation that can be verified case by case. Also, the statement should be written with the notion of 'stable traveling waves', because traveling waves can also connect an unstable state to a Turing unstable state [26]. However, they are unstable in the sense that the dynamic creates periodic patterns.

Proof of Theorem 7.1 We consider the Laplace operator, with a Dirichlet or a Neumann condition according to those considered for the system (7.4). It has an orthonormal basis of eigenfunctions $(w_k)_{k\geq 1}$ associated with positive eigenvalues λ_k,

$$-\Delta w_k = \lambda_k w_k.$$

We recall that we know that $\lambda_k \xrightarrow[k\to\infty]{} \infty$. We use this basis to decompose $u(t)$ and $v(t)$, i.e.,

$$u(t) = \sum_{k=1}^{\infty} \alpha_k(t)\, w_k, \qquad v(t) = \sum_{k=1}^{\infty} \beta_k(t)\, w_k.$$

We can project the system (7.4) on these eigenfunctions and arrive to

$$\begin{cases} \frac{d\alpha_k(t)}{dt} + \sigma_u \lambda_k \alpha_k(t) = a\alpha_k(t) + b\beta_k(t), \\ \frac{d\beta_k(t)}{dt} + \sigma_v \lambda_k \beta_k(t) = c\alpha_k(t) + d\beta_k(t). \end{cases} \tag{7.5}$$

Now, we look for solutions with exponential growth in time, i.e., $\alpha_k(t) = e^{\lambda t}\overline{\alpha}_k$, $\beta_k(t) = e^{\lambda t}\overline{\beta}_k$ with $\lambda > 0$ (in fact a complex number with $Re(\lambda) > 0$ is sufficient, but this does not change the conditions we find below). The system is again reduced to

$$\begin{cases} \lambda\, \overline{\alpha}_k + \sigma_u \lambda_k \overline{\alpha}_k = a\overline{\alpha}_k + b\overline{\beta}_k, \\ \lambda\, \overline{\beta}_k + \sigma_v \lambda_k \overline{\beta}_k = c\overline{\alpha}_k + d\overline{\beta}_k. \end{cases} \tag{7.6}$$

This is a $2 * 2$ linear system for $\overline{\alpha}_k$, $\overline{\beta}_k$ and it has a nonzero solution if, and only if, its determinant vanishes

$$0 = \det \begin{pmatrix} \lambda + \sigma_u \lambda_k - a & -b \\ -c & \lambda + \sigma_v \lambda_k - d \end{pmatrix}$$

Hence, there is a solution with exponential growth for those eigenvalues λ_k for which

$$\text{there is a root } \lambda > 0 \text{ to } (\lambda + \sigma_u \lambda_k - a)(\lambda + \sigma_v \lambda_k - d) - bc = 0. \tag{7.7}$$

This condition can be further reduced to the *dispersion relation*

$$\lambda^2 + \lambda\big[(\sigma_u + \sigma_v)\lambda_k - \mathcal{T}\big] + \sigma_u\, \sigma_v (\lambda_k)^2 - \lambda_k(d\, \sigma_u + a\, \sigma_v) + \mathcal{D} = 0.$$

Because the first order coefficient of this polynomial is positive, it can have a positive root if, and only if, the zeroth order term is negative

$$\sigma_u\, \sigma_v (\lambda_k)^2 - \lambda_k(d\, \sigma_u + a\, \sigma_v) + \mathcal{D} < 0,$$

and we arrive to the final condition

$$(\lambda_k)^2 - \lambda_k\left(\frac{d}{\sigma_v} + \frac{a}{\sigma_u}\right) + \frac{\mathcal{D}}{\sigma_u \sigma_v} < 0. \tag{7.8}$$

Because $\lambda_k > 0$ and $\frac{\mathcal{D}}{\sigma_u \sigma_v} > 0$, this polynomial can take negative values only for $\frac{d}{\sigma_v} + \frac{a}{\sigma_u} > 0$ and sufficiently large, with $\frac{\mathcal{D}}{\sigma_u \sigma_v}$ sufficiently small. It is difficult to give an accurate general characterization in terms of σ_u and σ_v when (a, b, c, d) are fixed because we do not know, in general, the distribution of the eigenvalues.

To go further, we set

$$\theta = \frac{\sigma_u}{\sigma_v},$$

and we write explicitly the roots of the above polynomial and we require that

$$\lambda_k \in [\Lambda_-, \Lambda_+], \qquad \Lambda_\pm = \frac{1}{2\sigma_v \theta}\left[d\theta + a \pm \sqrt{\left(d\theta + a\right)^2 - 4\mathcal{D}\theta}\,\right]. \tag{7.9}$$

We can restrict ourselves to the regime θ small, then the Taylor expansion gives,

$$\Lambda_\pm = \frac{d\theta + a}{2\sigma_v \theta}\left[1 \pm \sqrt{1 - \frac{4\mathcal{D}\theta}{(d\theta + a)^2}}\,\right],$$

$$\Lambda_{\pm} \approx \frac{a}{2\sigma_v \theta}\left[1 \pm [1 - \frac{2\mathcal{D}\theta}{(d\theta + a)^2}]\right],$$

and thus

$$\Lambda_{-} \approx \frac{\mathcal{D}}{a\,\sigma_v} = O(1), \qquad \Lambda_{+} \approx \frac{a}{\sigma_v \theta} \gg 1.$$

In the regime σ_u small, σ_v of the order of 1, the interval $[\Lambda_-, \Lambda_+]$ becomes very large, hence we know that some eigenvalues λ_k will belong to this interval.

Note however that, because $\lim_{k\to\infty} \lambda_k = +\infty$, there are only a finite number of unstable modes λ_k. □

In principle one will observe the mode w_{k^0} corresponding to the largest possible λ in (7.7) among the λ_k's that satisfy the condition (7.9). This does not correspond necessarily to the largest value of λ_k that satisfy the inequality (7.8).

Exercise Compute the first two terms in the expansion of λ in $\lambda_k \to \infty$.

Solution $\lambda \approx -\sigma_u \lambda_k + \mathcal{T}$.

Exercise Check how the condition (7.8) is generalized if we only impose the more general instability criteria that (7.7) holds with $\lambda \in \mathbb{C}$ and $Re(\lambda) > 0$.

7.2 Spots on the Body and Stripes on the Tail

Several papers [30] and [18] (see also [25]) give a striking explanation of how Turing instability provides us with a possible explanation of why so many animals have spots on the body and stripes on the tail, see Fig. 7.1. In short, in a long and narrow domain (a tail), typical eigenfunctions are 'bands', and with a more spherically shaped domain (a mathematical square body), the eigenfunctions are 'spots' or 'chessboards'. A much better and more detailed discussion with precise

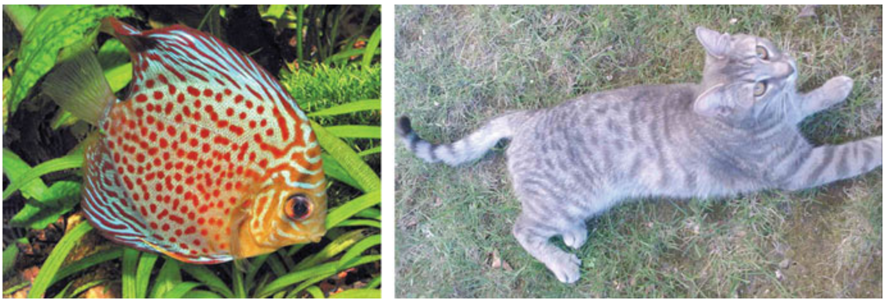

Fig. 7.1 Examples of animals with spots and stripes. *Left*: Discus (http://animal-world.com/encyclo/fresh/cichlid/discus.php). *Right*: My cat

biological cases demonstrated, and also the original papers where this idea is first expressed, can be found in [25] Vol. II, Chapter 3.

To explain this, we consider the Neumann boundary condition and use our computations of eigenvalues from Sect. 2.5.2. In one dimension, in a domain $[0, L]$, the eigenvalues and eigenfunctions are

$$\lambda_k = \left(\frac{\pi k}{L}\right)^2, \qquad w_k(x) = \cos\left(\frac{\pi k x}{L}\right), \qquad k \in \mathbb{N}.$$

In a rectangle $[0, L_1] \times [0, L_2]$, we obtain the eigenelements, for $k, l \in \mathbb{N}$

$$\lambda_{kl} = \left(\frac{\pi k}{L_1}\right)^2 + \left(\frac{\pi l}{L_2}\right)^2, \qquad w_{kl}(x, y) = \cos\left(\frac{\pi k x}{L_1}\right) \cos\left(\frac{\pi l y}{L_2}\right).$$

Consider a narrow stripe, say $L_2 \approx 0$ and $L_1 \gg 1$. The condition (7.9), namely $\lambda_{kl} \in [\Lambda_-, \Lambda_+]$, will impose $l = 0$ otherwise λ_{kl} will be very large and cannot fit the interval $[\Lambda_-, \Lambda_+]$. The corresponding eigenfunctions are bands parallel to the y axis.

When $L_2 \approx L_1$, the distribution of sums of squared integers generically determines that the distribution of the $\lambda_{kl} \in [\Lambda_-, \Lambda_+]$ will be for $l \approx k$.

To conclude this section, we point out that growing domains during development also very strongly influence the topic of pattern formation. Again, we refer to [25] for a detailed analysis of the Turing patterns, and their interpretation in development biology.

7.3 The Simplest Nonlinear Example: The Non-local Fisher/KPP Equation

As a simple nonlinear example to explain what is Turing instability, we consider the non-local Fisher/KPP equation

$$\frac{\partial}{\partial t} u - \nu \frac{\partial^2}{\partial x^2} u = r\, u(1 - K * u), \qquad t \geq 0,\ x \in \mathbb{R}, \tag{7.10}$$

still with $\nu > 0$, $r > 0$, given parameters. For the convolution kernel K, we choose a smooth probability density function

$$K(\cdot) \geq 0, \qquad \int_R K(x) dx = 1, \qquad K \in L^\infty(\mathbb{R}) \quad \text{(at least)}.$$

Compared to the Fisher/KPP equation, this takes into account that competition for resources can be of long range (the size of the support of K) and not only local.

This idea has been proposed in ecology as an improvement of the Fisher equation that takes into account long range competition for resources (N.F. Britton [4] and

Gourley [10]). In semi-arid regions the roots of trees, in competition for water, can cover, up to ten times the external size of the tree itself (while in temperate regions the ratio is roughly one to one). This leads to the so-called 'tiger bush' landscape [15].

The same equation has also been proposed as a simple model of adaptive evolution. Then x represents a phenotypical trait, see S. Génieys et al. [8]. The Laplace term represents mutations and the right hand side, growth and competition. The convolution kernel is used to express that competition is higher between individuals, whose traits are close to each other (see also Sect. 5.1.2).

The convolution term has a drastic effect for solutions; it can induce solutions that exhibit a behavior quite different from those of the Fisher/KPP equation. The reason is mainly that the maximum principle is lost with the non-local term. Again, we notice that the steady state $u \equiv 0$ is unstable, that $u \gg 1$ is also unstable because it induces a strong decay. In one dimension, for a general reaction function $f(u)$ the conditions read $f(0) = 0, f'(0) > 0$ and $f(u) < 0$ for u large. Consequently there is a point u_0 satisfying (generically) $f(u_0) = 0, f'(u_0) < 0$, i.e. a stable steady state should be found between the unstable ones. This is the case of the nonlinearities arising in the Fisher/KPP equation that we have already encountered.

In the infinite dimensional framework at hand, we shall see that under certain circumstances, the steady state $u \equiv 1$ can be unstable in the sense of

Definition 7.2 The steady state $u \equiv 1$ is called *linearly unstable* if there are perturbations such that the linearized system has exponential growth in time.

Then, the following conditions are satisfied

Definition 7.3 A steady state u_0 is said to form Turing patterns if

(i) there is no blow-up, no extinction (it is between two unstable states as above),
(ii) it is linearly unstable,
(iii) the corresponding growth modes are bounded (no high frequency oscillations).

Obviously when Turing instability occurs, solutions should exhibit strange behavior because they remain bounded away from the two extreme steady states, they cannot converge to the steady state u^0 or oscillate rapidly. In other words, they should exhibit Turing patterns. See Fig. 7.2 for a numerical solution of (7.10).

In practice, to check linear instability we use a spectral basis. In compact domains the concept can be handled using eigenfunctions of the Laplace operator as we did in Sect. 7.1. In the full line, we may use the generalized eigenfunctions, these are the Fourier modes. We define the Fourier transform as

$$\hat{u}(\xi) = \int_{\mathbb{R}} u(x) e^{-ix\,\xi} dx.$$

Theorem 7.4 *Assume the condition*

$$\exists \xi_0 \quad \textit{such that } \hat{K}(\xi_0) < 0, \tag{7.11}$$

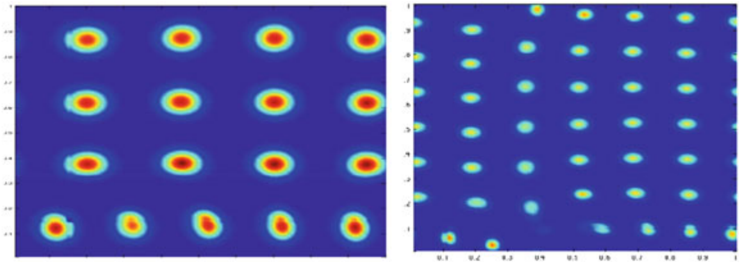

Fig. 7.2 Two steady state solutions of the non-local Fisher/KPP equation (7.10) in 2 dimensions with different diffusion coefficients

then, for ν/r sufficiently small (depending on ξ_0 and $K(\xi_0)$), the non-local Fisher/KPP equation (7.10) *is nonlinearly Turing unstable.*

A practical consequence of this theorem is that solutions should create Turing patterns as mentioned earlier. This can easily be observed in numerical simulations, see Fig. 7.2.

The non-local Fisher equation also gives an example of the already mentioned **Turing instability alternative**.

- Turing instability $\iff$ $K(\cdot)$ is long range.
- Traveling waves $\iff$ $K(\cdot)$ is short range.

Indeed the non-local term $K * u$ is the inhibitor (negative) term. The diffusion represents the activator (with a coefficient normalized to 1). The limit of very short range is the case of $K = \delta$, a Dirac mass, and we recover the Fisher/KPP equation. More on this is proved in [3].

Proof

(i) The state $u \equiv 0$ and $u \equiv \infty$ are indeed formally both unstable (to prove this rigorously is not so easy for $u \equiv \infty$).

(ii) The linearized equation around $u \equiv 1$ is obtained by setting $u = 1 + \tilde{u}$ and keeping the first order terms, we obtain

$$\frac{\partial}{\partial t}\tilde{u} - \nu \frac{\partial^2}{\partial x^2}\tilde{u} = -r\, K * \tilde{u}.$$

And we look for solutions of the form $\tilde{u}(t,x) = e^{\lambda t} v(x)$ with $\lambda > 0$. This means that we should find eigenfunctions associated with the positive eigenvalue λ, that means solution $v(x)$ of

$$\lambda v - \nu \frac{\partial^2}{\partial x^2} v = -r\, K * v.$$

We look for a possible Fourier mode $v(x) = e^{ix\,\xi_1}$ that we insert in the previous equation. Then we obtain the condition

$$\lambda + \nu\xi_1^2 = -r\,\hat{K}(\xi_1), \qquad \text{for some } \ \lambda > 0. \tag{7.12}$$

And it is indeed possible to obtain such a λ and a $\xi_1 = \xi_0$ under the conditions of the theorem.

(iii) The possible unstable modes ξ_0 are obviously bounded because $\hat{K}$ is bounded as the Fourier transform of a probability density ($|\hat{K}| \le 1$). □

Note however that the mode ξ_1 we observe in practice is that with the highest growth rate λ.

7.4 Phase Transition: What is NOT Turing Instability

What happens if the third condition in Definition 7.3 does not hold? The system remains bounded away from zero and infinity by condition (i) and it is unstable by condition (ii). But it might 'blow-up' by high frequency oscillations.

As an example of such an unstable system, which is not Turing unstable, we consider the phase transition model also used in Sect. 8.10,

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta A(u) = 0, \qquad x \in \Omega, \\ \\ \frac{\partial}{\partial \nu} u = 0 \qquad \text{on } \partial\Omega, \end{cases} \tag{7.13}$$

with

$$A(u) = u\,(3-u)^2. \tag{7.14}$$

Because $A'(u) = 3(3-u)(1-u) < 0$, Eq. (7.13) is a backward-parabolic equation in the interval $u \in (1,3)$. We expect that linear instability occurs in this interval. We take $\bar{u} = 2$ and set

$$u = 2 + \tilde{u},$$

Inserting this in the above equation we find the linearized equation for $\tilde{u}(t,x)$

$$\begin{cases} \frac{\partial \tilde{u}}{\partial t} - A'(2)\Delta\tilde{u} = 0, \qquad x \in \Omega, \\ \\ \frac{\partial}{\partial \nu}\tilde{u} = 0 \qquad \text{on } \partial\Omega. \end{cases}$$

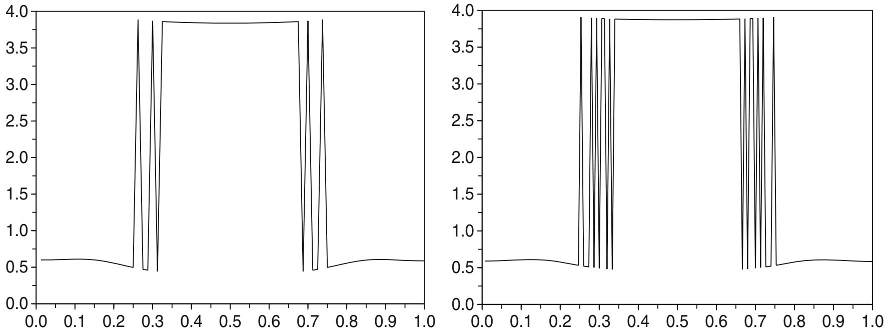

Fig. 7.3 Two numerical solutions of the phase transition system (7.13)–(7.14) for (*Right*) 80 grid points and (*Left*) 150 grid points. The oscillation frequencies depend on the grid and these are not Turing patterns

We set $\gamma = -A'(2) > 0$ and we look for solutions $\tilde{u}(t,x) = e^{\lambda t} w(x)$, which are unstable, i.e., $\lambda > 0$. These are given by

$$\lambda w + \gamma \Delta w = 0,$$

and thus they stem from the Neumann eigenvalue problem in Theorem 2.7. We have

$$\lambda = \lambda_i \gamma, \qquad w = w_i.$$

We can see that all the eigenvalues of the Laplace operator generate possible unstable modes and thus they can be of very high frequency. And we expect to see the mode corresponding to the largest λ, i.e., to the largest λ_i which of course does not exist because $\lambda_i \underset{i\to\infty}{\longrightarrow} \infty$. In the space variable these correspond to highly oscillatory eigenfunctions w_i that we can observe numerically.

Figure 7.3 gives numerical solutions of (7.13)–(7.14) corresponding to two different grids; high frequency solutions are obtained that depend on the grid. This defect explains why we require bounded unstable modes in the definition of Turing instability. It also explains why in Sect. 8.10 we have introduced a relaxation system.

More on the subject of phase transitions can be found in Chap. 10 on the Stefan problem.

7.5 Gallery of Parabolic Systems Giving Turing Patterns

Many examples of nonlinear parabolic systems exhibiting Turing instabilities (and patterns) have been widely studied. This section gives several examples but it is in no way complete; the theories are far too complicated to be presented here and their use in biology and other applications are far too numerous.

7.5.1 A Cell Polarity System

We take the following system from Morita and Ogawa [23]

$$\begin{cases} \frac{\partial}{\partial t}u - \sigma_1 \Delta u = -f(u) + v, & t \geq 0, \ x \in \Omega, \\ \frac{\partial}{\partial t}v - \sigma_2 \Delta v = \quad f(u) - v, & \\ u(x,t) = v(x,t) = 0 \quad \text{sur } \ \partial\Omega. & \end{cases} \tag{7.15}$$

We take a function $f \in C^2(\mathbb{R}^+; \mathbb{R}^+)$ that, for a given value $u_c > 0$, satisfies

$$f(0) = 0, \quad f'(u) > 0 \text{ for } u \in [0, u_c[, \quad -1 < f'(u) < 0 \text{ for } u > u_c, \quad f(+\infty) = 0.$$

This system is mass conservative since one can prove that

$$u(t,x) > 0, \quad v(t,x) > 0, \qquad \frac{d}{dt}\int_\Omega [u(t,x) + v(t,x)]dx = 0.$$

These properties give us the non-extinction/non-blow-up conditions.

We analyze Turing instability.

The Differential System is Stable The corresponding differential system is

$$\begin{cases} \frac{d}{dt}U = -f(U) + V, & t \geq 0, \\ \frac{d}{dt}V = \quad f(U) - V, & \\ U(0) > 0, \quad V(0) > 0. & \end{cases}$$

It satisfies $U(t) + V(t) = U(0) + V(0) =: M^0 > 0$ and thus can be also written as

$$\frac{d}{dt}U = -f(U) + M^0 - U(t) := G(U(t)).$$

Therefore, it preserves the positive cone

$$U(t) > 0, \qquad V(t) > 0,$$

indeed, at the first point t_0 where $u(t_0) = 0$ we have $\frac{d}{dt}U(t_0) = M^0 > 0$, which cannot be correct (same argument to handle the function V).

Since $G'(u) = -f'(u) - 1 < 0$, $G(0) > 0$ and $G(+\infty) = -\infty$, there is a single steady state $(\bar{u}, \bar{v})$ characterized by $G(\bar{u}) = 0$ that is equivalent to

$$\bar{u} + \bar{v} = M^0, \qquad \bar{v} = f(\bar{u}). \tag{7.16}$$

Because $G(U) > 0$ for $U \leq \bar{u}$, $G(U) < 0$ for $U \geq \bar{u}$, it is very clear that (monotonically)

$$U(t) \underset{t\to\infty}{\longrightarrow} \bar{u}, \qquad V(t) \underset{t\to\infty}{\longrightarrow} \bar{v}.$$

Turing Instability Consider a steady state (7.16). We compute the differential matrix for the right hand side

$$\begin{pmatrix} -f'(\bar{u}) & 1 \\ f'(\bar{u}) & -1 \end{pmatrix}$$

To fit the assumptions of Theorem 7.1, we have to check $\mathcal{T} := -f'(\bar{u})-1 < 0, \mathcal{D} := 0$ (a degenerate case, corresponding to mass conservation). The only possibility is that u is the activator, which imposes

$$f'(\bar{u}) < 0 \iff \bar{u} > u_c.$$

Then, we find that unstable modes $e^{\lambda t}(\alpha w_k, \beta w_k)$ exist if there is a positive root to the polynomial

$$\lambda^2 + \lambda[\lambda_k(\sigma_1 + \sigma_2) + f'(\bar{u}) + 1] + (\sigma_1\lambda_k + f'(\bar{u}))(\sigma_2\lambda_k + 1) - f'(\bar{u}) = 0.$$

As in Sect. 7.1, this is equivalent to

$$(\sigma_1\lambda_k + f'(\bar{u}))(\sigma_2\lambda_k + 1) - f'(\bar{u}) = \sigma_1\sigma_2\lambda_k^2 + \sigma_1\lambda_k + \sigma_2 f'(\bar{u})\lambda_k < 0,$$

$$\lambda_k + \frac{1}{\sigma_2} \leq \frac{|f'(\bar{u})|}{\sigma_1}.$$

This is clearly satisfied for some eigenvalues λ_k when σ_1 is sufficiently small; this is the same result as in Theorem 7.1.

7.5.2 The CIMA Reaction

As mentioned earlier, the first experimental evidence of Turing instability was obtained with the CIMA (chlorite-iodide-malonic acid) chemical reaction. It was modeled by I. Lengyel and I.R. Epstein [16] who proposed the system (with $c = 1$)

$$\begin{cases} \dfrac{\partial u}{\partial t} - \sigma_u \Delta u = a - u - \dfrac{4uv}{1+u^2}, \\ \dfrac{\partial v}{\partial t} - \sigma_v \Delta v = bc\, u - \dfrac{cuv}{1+u^2}. \end{cases} \tag{7.17}$$

Here u (the activator) denotes the iodide (I^-) concentration and v (the inhibitor) the chlorite (ClO_2^-) concentration. Existence of steady states was analyzed [27, 35].

Here we consider this system with $a > 0$, $b > 0$, $c > 0$. There is a single homogeneous steady state

$$\bar{u} = \frac{a}{4b+1}, \qquad \bar{v} = b(1+\bar{u}^2).$$

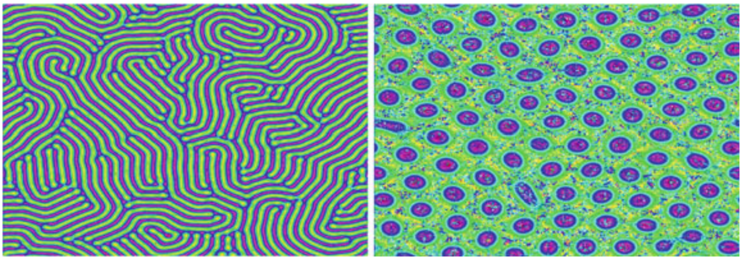

Fig. 7.4 Labyrinth and spot patterns in the CIMA reaction (7.17). The solutions have been computed with the software FreeFEM++ [7, 12] by S. Kaber

The simple invariant region for solutions (that means the bounds are satisfied for all times if initially true) are given by the maximum principle

$$0 \le u \le a, \qquad b \le v \le b(1+a^2) := v_M.$$

Also solutions cannot become extinct because we can use the upper bound on v to go further and find

$$u \ge u_{\min}, \qquad u_{\min}\Big(1+\frac{4v_M}{1+u_{\min}^2}\Big) = a,$$

(in fact we can go even further and find a more restrictive invariant region, iterating the argument). These a priori bounds are consequences of the maximum principle and we skip the derivation.

Therefore, according to our theory of Turing patterns, solutions cannot become extinct or blow-up (Fig. 7.4) and it remains to study the linearized operator around the steady state $(\bar{u}, \bar{v})$.

Lemma 7.5 *The CIMA reaction system* (7.17) *is Turing unstable if*

$$4b > 1, \qquad c > 2\sqrt{16b^2-1}, \qquad \sqrt{\frac{4b+1}{4b-1}} < \bar{u} < \frac{c+\sqrt{c^2-4(16b^2-1)}}{2(4b-1)},$$

and u is the activator, v the inhibitor.

Consequently, for this range of parameters, σ_v of the order of 1, and σ_u sufficiently small, there will be Turing patterns.

With the first two conditions for b and c, because $\frac{c+\sqrt{c^2-4(16b^2-1)}}{2(4b-1)} > \sqrt{\frac{4b+1}{4b-1}}$, the third set of inequalities is a condition to ensure that a is not too small, neither too large.

Proof We compute the differential matrix for the right hand side

$$\begin{pmatrix} -1-4\bar{v}\frac{1-\bar{u}^2}{(1+\bar{u}^2)^2} & -\frac{4\bar{u}}{1+\bar{u}^2} \\ bc-c\bar{v}\frac{1-\bar{u}^2}{(1+\bar{u}^2)^2} & -\frac{c\bar{u}}{1+\bar{u}^2} \end{pmatrix} = \begin{pmatrix} -1-\frac{4b^2}{\bar{v}}(1-\bar{u}^2) & -\frac{4b\bar{u}}{\bar{v}} \\ bc-\frac{cb^2}{\bar{v}}(1-\bar{u}^2) & -\frac{cb\bar{u}}{\bar{v}} \end{pmatrix}$$

Using Theorem 7.1, and because the bottom right coefficient is negative, we have to check the conditions

$$-1-\frac{4b^2}{\bar{v}}(1-\bar{u}^2)>0, \qquad \mathcal{T}r=-1-\frac{4b^2}{\bar{v}}(1-\bar{u}^2)-\frac{cb\bar{u}}{\bar{v}}<0,$$

$$\mathcal{D}et=(1+\frac{4b^2}{\bar{v}}(1-\bar{u}^2))\frac{cb\bar{u}}{\bar{v}}+\frac{4b\bar{u}}{\bar{v}}(bc-\frac{cb^2}{\bar{v}}(1-\bar{u}^2))=\frac{cb\bar{u}}{\bar{v}}+\frac{4cb^2\bar{u}}{\bar{v}}>0.$$

The condition on the determinant is always satisfied. The only constraints on a, b, c come from the first line. Replacing $\bar{v}$ by its value, we need first

$$4b^2\bar{u}^2-4b^2-b(1+\bar{u}^2)>0 \iff \bar{u}^2>\frac{4b+1}{4b-1}.$$

Secondly, the trace condition gives

$$(4b-1)\bar{u}^2-c\bar{u}-(4b+1)<0 \Longrightarrow \frac{c-\sqrt{c^2-4(16b^2-1)}}{2(4b-1)}<\bar{u}$$
$$<\frac{c+\sqrt{c^2-4(16b^2-1)}}{2(4b-1)},$$

which is the announced condition.

A subtle calculation that is left to the reader shows that $\sqrt{\frac{4b+1}{4b-1}} > \frac{c-\sqrt{c^2-4(16b^2-1)}}{2(4b-1)}$ and thus the statement is proved.

Then one can assert that for $\sigma_u \ll \sigma_v$, Turing patterns will be produced (in accordance with Theorem 7.1). □

7.5.3 The Diffusive Fisher/KPP System

The simplest system we have encountered so far is the diffusive Fisher/KPP system already mentioned in Sect. 4.9. It reads

$$\begin{cases} \frac{\partial u}{\partial t}-d_u\Delta u=g(u)v, \\ \frac{\partial v}{\partial t}-d_v\Delta v=-g(u)v. \end{cases} \tag{7.18}$$

For $d_u = d_v$, the solution $v = 1-u$ reduces (7.18) to the Fisher equation (4.1) with $f(u) = g(u)(1-u)$. Therefore, this system still exhibits traveling waves. It has been proved that even for $d_v \neq d_u$, the system has monotonic traveling waves [2, 17, 20] for a power law nonlinearity $g(u) = u^n$.

From the Turing instability alternative in Sect. 7.1, we do not expect Turing patterns at this stage. This is why interesting examples are always a little more elaborate.

Exercise Consider the steady states $(U = \gamma, V = 0)$, $\gamma > 0$ of (7.18) with $g(u) = u^n$.

1. Compute the linearized equation around this steady state.
2. In the whole space or a bounded domain with a Neumann boundary condition, show that this steady state is always stable.

7.5.4 The Brusselator

Prigogine and Lefever [31] and Nicolis and Prigogine [29] proposed an example now called the Brusselator. This is certainly the simplest system exhibiting Turing patterns; see also Sects. 7.5.5 and 7.5.6.

Let $A > 0, B > 0$ be given positive real numbers. In a finite domain Ω, we consider the following $2 \star 2$ system with a Neumann boundary condition

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = A - (B+1)u + u^2 v, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = Bu - u^2 v. \end{cases} \tag{7.19}$$

We check below that there is a single positive steady state that exhibits the linear conditions for Turing instability. Also the solution cannot vanish, thanks to the term $A > 0$. But we are not aware of a proof that the solutions remain bounded for t large.

Exercise

1. Check that the only homogeneous steady state is $(U = A, V = \frac{B}{A})$.
2. Write the linearized system around this steady state.
3. Check that for $B < 1 + A^2$, this steady state is attractive for the associated differential equation ($d_u = d_v = 0$).
4. Let $d_u > 0,\ d_v > 0$ and consider an eigenpair (λ_i, w_i) of the Laplace equation with a Neumann boundary condition. Write the condition for A, B, d_u, d_v, λ_i for which there is an unstable mode $\lambda > 0$.
5. Show that for $\theta := \frac{d_u}{d_v} < 1$ the interval $[\Lambda_-, \Lambda_+]$ for λ_i is not empty.
6. Show that for θ small we have $\Lambda_- \approx \frac{A^2}{d_v}$, $\Lambda_+ \approx \frac{B-1}{2 d_v \theta}$. Conclude that for d_v fixed and d_u small, the steady state becomes unstable.

Solution 2.

$$\begin{cases} \frac{\partial \tilde{u}}{\partial t} - d_u \Delta \tilde{u} = (B-1)\tilde{u} + A^2 \tilde{v}, \\ \frac{\partial \tilde{v}}{\partial t} - d_v \Delta \tilde{v} = -B\tilde{u} - A^2 \tilde{v}. \end{cases}$$

3. $det = A^2$, $tr = B - 1 - A^2$ and see Sect. 7.1 for the condition $tr < 0$, which leads to $B < 1 + A^2$.
4. As in the general theory, we arrive to a second order polynomial for λ, which implies that the constant term should be negative, leading to the condition

$$d_u d_v \lambda_i^2 + \lambda_i (A^2 d_u - (B-1) d_v) + A^2 < 0.$$

5. To have two positive roots, we need a negative slope at the origin, i.e., $B > 1 + \frac{d_u}{d_v} A^2$ and also

$$(B-1)d_v - A^2 d_u > 2A\sqrt{d_u\, d_v} \iff B > 1 + 2\sqrt{\theta} A + \theta A^2.$$

This is compatible with the condition of question 3 if, and only if, $\theta < 1$.

6. We have

$$\Lambda_\pm = \frac{1}{2 d_v \theta}[B - 1 - A^2\theta \pm \sqrt{(B - 1 - A^2\theta)^2 - 4A^2\theta}\ ].$$

The Taylor expansion for θ small reads

$$\Lambda_\pm = \frac{1}{2 d_v \theta}(B - 1 - A^2\theta)\left[1 \pm \sqrt{1 - \frac{4A^2\theta}{(B - 1 - A^2\theta)^2}}\ \right]$$

$$\Lambda_\pm \approx \frac{1}{2 d_v \theta}(B - 1 - A^2\theta)\left[1 \pm (1 - \frac{2A^2\theta}{(B - 1 - A^2\theta)^2})\ \right]$$

and thus

$$\Lambda_- \approx \frac{A^2}{d_v}, \qquad \Lambda_+ \approx \frac{B-1}{d_v \theta}.$$

For d_v fixed and θ small this interval will contain eigenvalues λ_i.

The two parabolic regions in (A, B) are drawn in Figs. 7.5 and 7.6.

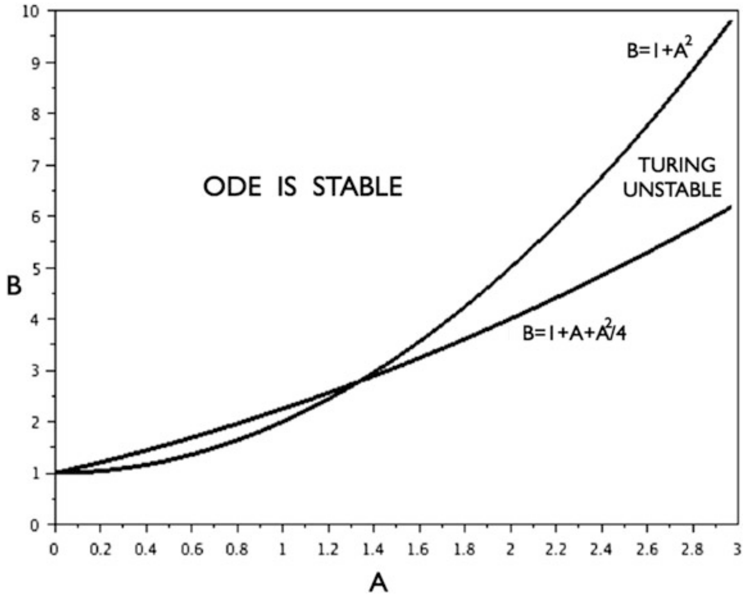

Fig. 7.5 The Turing instability region of the brusselator in the (A, B) plane

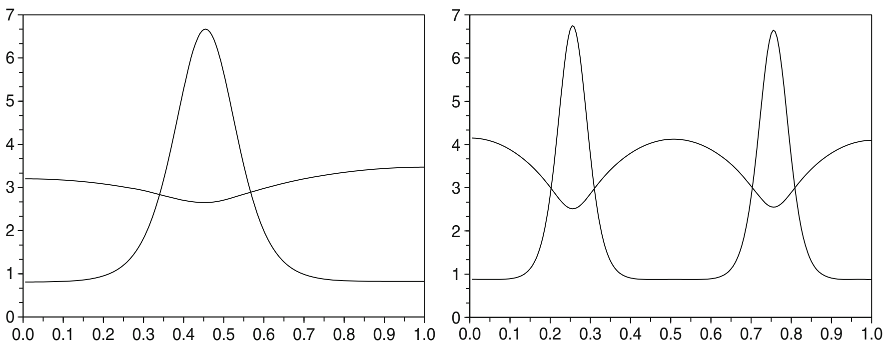

Fig. 7.6 Two numerical solutions of the brusselator system (7.19) with $A = B = 2$ and 200 grid points. The choice of diffusion coefficients are (*Left*) $d_v = 1.$ and $d_u = 0.005$ (*Right*) $d_v = 0.1$ and $d_u = 0.001$. The first component u exhibits one or two strong peak(s) upward while v exhibits one or two minimum(s) and has been magnified by a factor 5

7.5.5 The Gray-Scott System (2)

Gray and Scott [11] introduced this system as a model of a chemical reaction between two constituents. It only differs from the Brusselator (7.19) by a change in the constant coefficients of the reaction term

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u^n v - Au, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = -u^n v + B(1-v). \end{cases} \tag{7.20}$$

Again $A > 0$, $B \geq 0$ are constants (input, degradation of constituents) and n is an integer, which determines the number of molecules u which react with a single molecule v.

The system (7.20) differs from the Brusselator (7.19) in that it is bistable. To explain this, we only consider the case

$$n = 2, \qquad B > 4A^2. \tag{7.21}$$

We first notice that there are three homogeneous steady states to the Gray-Scott system; the trivial one ($U_0 = 0, V_0 = 1$) and non-vanishing ones $(U_\pm, V_\pm)$, given by

$$UV = A, \qquad AU = B(1-V).$$

We can eliminate V or U and find $AU^2 - BU + AB = 0$ and $BV^2 - BV + A^2 = 0$, this means that

$$U_\pm = \frac{B \pm \sqrt{B^2 - 4A^2B}}{2A}, \quad V_\pm = \frac{B \mp \sqrt{B^2 - 4A^2B}}{2B}. \tag{7.22}$$

It is easy (but tedious) to see that the following results hold:

Lemma 7.6 *With the assumption* (7.21)*, the steady state* (U_-, V_-) *is linearly unstable, the state* $(U_0 = 0, V_0 = 1)$ *is linearly stable and* (U_+, V_+) *is linearly stable under the additional condition* (7.23) *below.*

Proof The linearized systems read

$$\begin{cases} \frac{\partial \tilde{u}}{\partial t} = (2UV - A)\tilde{u} + U^2 \tilde{v}, \\ \frac{\partial \tilde{v}}{\partial t} = -2UV\tilde{u} - (U^2 + B)\tilde{v}. \end{cases}$$

We begin with the trivial steady state (U_0, V_0). Together with the general analysis of Sect. 7.1, we compute, for the trivial steady state, the quantities

$$\mathcal{D}_0 = AB > 0, \qquad \mathcal{T} = -A - B < 0.$$

This means that for the steady state (U_0, V_0), the corresponding O.D.E. system is linearly attractive.

For the non-vanishing ones, using the above rule $UV = A$, we also compute

$$\begin{cases} \frac{\partial \tilde{u}}{\partial t} = A\tilde{u} + U^2\tilde{v}, \\ \frac{\partial \tilde{v}}{\partial t} = -2A\tilde{u} - (U^2 + B)\tilde{v}, \end{cases}$$

$$\mathcal{D} = A(U^2 - B) > 0, \qquad \mathcal{T} = A - B - U^2.$$

We deduce from (7.22)

$$\begin{aligned} U_\pm^2 - B &= \tfrac{B^2}{2A^2} - 2B \pm \tfrac{B}{2A^2}\sqrt{B^2 - 4A^2B} \\ &= \tfrac{B}{2A^2}\left[B - 4A^2 \pm \sqrt{B^2 - 4A^2B}\right]. \end{aligned}$$

Therefore, obviously $\mathcal{D}_+ > 0$ and

$$\mathcal{D}_- = \frac{B}{2A^2}\sqrt{B^2 - 4A^2B}\left[\sqrt{B - 4A^2} - \sqrt{B}\right] < 0.$$

Therefore, for the steady state (U_-, V_-), the corresponding O.D.E. system is unstable.

It remains to check the trace condition for (U_+, V_+). We have

$$\mathcal{T} = A - \frac{B^2}{2A^2} - \frac{B}{2A^2}\sqrt{B^2 - 4A^2B} < 0, \tag{7.23}$$

which is an additional condition to be checked. Note that, for the limiting value $B = 4A^2$, this inequality means that $A > 1/8$. Therefore, it is clearly compatible with (7.21). □

We can now come back to the traveling wave solutions. We consider the particular case $d_u = d_v$, $A = B$ and choosing $v(t,x) = 1 - u(t,x)$. Then, the two equations of (7.20) reduce to the single equation

$$\frac{\partial u}{\partial t} - d_u\Delta u = u^2(1-u) - Au = u(u - u^2 - A).$$

This is the situation of the Allen-Cahn (bistable) equation where, for A sufficiently small, we have three steady states $U_0 = 0$ is stable, U_- is unstable and $U_+ > U_- > 0$ is stable. Therefore, we have indeed a unique traveling wave solution (see Sect. 4.7). C.B. Mratov and V.V. Ospinov [24] develop an extended study of traveling waves in Gray-Scott system.

7.5.6 Schnakenberg System

The Schnakenberg system [32] is still another variant of the Brusselator (7.19) and the Gray-Scott system (7.20) with a constant input in the reaction terms. It is written as

$$\begin{cases} \frac{\partial u}{\partial t} - d_u \Delta u = C + u^2 v - Au, \\ \frac{\partial v}{\partial t} - d_v \Delta v = B - u^2 v. \end{cases} \tag{7.24}$$

With $C = 0$, it has been advocated by T. Kolokolnikov et al. [13] as a simple model for spot-pattern formation and spot-splitting in the following asymptotic regime

$$\begin{cases} \frac{\partial u}{\partial t} - \varepsilon \Delta u = u^2 v - Au, \\ \varepsilon \frac{\partial v}{\partial t} - d_v \Delta v = B - \frac{u^2 v}{\varepsilon}. \end{cases} \tag{7.25}$$

The scaling has the advantage to show explicitly the connection with Theorem 7.1, u is the activator, v the inhibitor in the linearized system around $\overline{u} = \frac{B}{A\varepsilon}$, $\overline{v} = \frac{A^2\varepsilon}{B}$.

7.5.7 The FitzHugh-Nagumo System with Diffusion

Consider again the FitzHugh-Nagumo system as already studied in Sect. 5.2.2, but with diffusion for both components,

$$\begin{cases} \frac{\partial u}{\partial t} - d_u \Delta u = u(1-u)(u - \frac{1}{2}) - v, \\ \frac{\partial v}{\partial t} - d_v \Delta v = \mu u - v, \end{cases} \tag{7.26}$$

with a Neumann boundary conditions.

Assume that

$$\mu > (1-u)(u - \frac{1}{2}) \qquad \forall u \in \mathbb{R}.$$

Then the only homogeneous steady state is $(0, 0)$ and this is stable for the associated differential equation.

Exercise We fix $d_v > 0$. Show that when d_u is sufficiently small, the steady state is unstable.

As already mentioned, there are many variants, one of them is

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u(1-u)(u-\alpha) - \beta uv, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = \gamma uv - \delta v(1-v). \end{cases} \tag{7.27}$$

This relates prey-predator systems and FitzHugh-Nagumo systems. See Sect. 7.6.3.

7.5.8 The Gierer-Meinhardt System

The Gierer-Meinhardt [9, 21, 22] system is one of the most famous examples exhibiting Turing instability and Turing patterns. It can be considered as a model for chemical reactions with only two reactants denoted by $u(t,x)$ and $v(t,x)$.

$$\begin{cases} \frac{\partial}{\partial t} u(t,x) - d_1 \Delta u(t,x) + Au = u^p/v^q, \quad t \geq 0,\ x \in \Omega, \\ \frac{\partial}{\partial t} v(t,x) - d_2 \Delta v(t,x) + Bv = u^r/v^s, \end{cases} \tag{7.28}$$

with a Neumann boundary condition.

Among this class, several authors have used the particular case with a single parameter

$$\begin{cases} \frac{\partial}{\partial t} u(t,x) - d_1 \Delta u(t,x) + Au = u^2/v, \quad t \geq 0,\ x \in \Omega, \\ \frac{\partial}{\partial t} v(t,x) - d_2 \Delta v(t,x) + v = u^2. \end{cases} \tag{7.29}$$

The diffusion coefficients satisfy

$$d_1 \ll 1 \ll d_2.$$

A possible limit is $d_2 \to \infty$, $v \to$ *constant* and thus we arrive to the reduced system for a steady state

$$\begin{cases} -\varepsilon^2 \Delta u + u = u^p, \qquad x \in \Omega, \\ \frac{\partial u}{\partial \nu} = 0 \qquad on\ \partial\Omega. \end{cases} \tag{7.30}$$

Following Berestycki and Lions [1], when $p < \frac{d+2}{d-2}$, there is a unique radial spike like solution $u = u_0(\frac{x}{\varepsilon})$ with

$$-\Delta u_0 + u_0 = u_0^p, \qquad x \in \mathbb{R}^d, \qquad u_0 > 0. \tag{7.31}$$

But in a bounded domain, see [19] there are solutions concentrating on the boundary $\partial\Omega$ without limitation on p.

Also for nonlinear systems of elliptic equations, there is a large literature, see J. Wei et al. [28, 34] and the references therein. They show that there are numerous types of solutions, and that they may undergo concentration properties in the case

$$\begin{cases} -\varepsilon^2 \Delta u + u = \frac{u^2}{v}, & x \in \mathbb{R}, \\ -\Delta v + v = u^2. \end{cases} \tag{7.32}$$

7.6 Models from Ecology

There are many standard models from ecology. The simplest versions never satisfy the conditions for Turing instability and we review some such examples first. Then we conclude with a more elaborate model which satisfies the Turing conditions for instability.

7.6.1 Competing Species and Turing Instability

Let us come back to models of competing species as already mentioned in Sect. 4.10. Let the coefficients r_1, r_2, α_1 and α_2 be positive in the system

$$\begin{cases} \frac{\partial}{\partial t} u_1 - d_1 \Delta u_1 = r_1 u_1 (1 - u_1 - \alpha_2 u_2), \\ \\ \frac{\partial}{\partial t} u_2 - d_2 \Delta u_2 = r_2 u_2 (1 - \alpha_1 u_1 - u_2). \end{cases} \tag{7.33}$$

We have seen in Sect. 4.10 that the positive steady state (U_1, U_2) is stable if, and only if, $\alpha_1 < 1, \alpha_2 < 1$. As stated in Theorem 7.1, to be Turing unstable, we require that one of the diagonal coefficients is positive in the linearized matrix

$$L = \begin{pmatrix} -r_1 U_1 & -\alpha_2 r_1 U_1 \\ \\ -\alpha_1 r_2 U_2 & -r_2 U_2 \end{pmatrix}$$

We see this is not the case. There is no activator in such systems.

7.6.2 Prey-Predator System

In system (7.33), we can also consider a prey-predator situation where $\alpha_1 < 0$ (u_1 is the prey) and $0 < \alpha_2 < 1$ (u_2 is the predator). With these conditions, the positive steady state is given by

$$(U_1, U_2) = \left(\frac{1 - \alpha_2}{1 - \alpha_2 \alpha_1}, \frac{1 - \alpha_1}{1 - \alpha_2 \alpha_1} \right).$$

Because

$$tr(L) = -(r_1 U_1 + r_2 U_2) < 0, \qquad det(L) = r_1 r_2 U_1 U_2 (1 - \alpha_1 \alpha_2) > 0,$$

this steady state is stable.

Again, according to Theorem 7.1, it cannot be Turing unstable because both diagonal coefficients are negative.

7.6.3 Prey-Predator System with Turing Instability (Problem)

Consider the prey-predator system (and see Sect. 7.5.7 for variants)

$$\begin{cases} \frac{\partial}{\partial t} u - d_u \Delta u = u(1 + u - \gamma \frac{u^2}{2} - \beta v), \\ \frac{\partial}{\partial t} v - d_v \Delta v = v(1 - v + \alpha u). \end{cases} \tag{7.34}$$

The purpose of the problem is to show there are parameters $\alpha > 0$, $\beta > 0$, $\gamma > 0$ for which Turing instability occurs. We assume

$$\beta < 1, \qquad \alpha\beta < 1.$$

1. Show there is a unique homogeneous stationary state ($\bar{u} > 0, \bar{v} > 0$). Show that

$$\gamma \bar{u} > 2(1 - \alpha\beta).$$

2. Compute the linearized matrix A of the differential system around this stationary state.
3. Compute the trace of A and show that $Tr(A) < 0$ if, and only if, the following condition is satisfied : $\bar{u}[1 - \alpha - \gamma \bar{u}] < 1$.
4. Compute the determinant of A and show that $Det(A) > 0$.
5. Which sign condition is also required for one of the coefficients of this matrix? How is it written in terms of $\gamma \bar{u}$?
6. Suppose also that $\alpha\beta > \frac{1}{2}$, $\alpha > 1$. Show that the above conditions are satisfied for γ sufficiently small.
7. For coefficients as in 6, state a Turing instability result concerning d_u, d_v.

Figure 7.7 shows a one dimensional numerical simulation of the system (7.34) in the Turing instability regime.

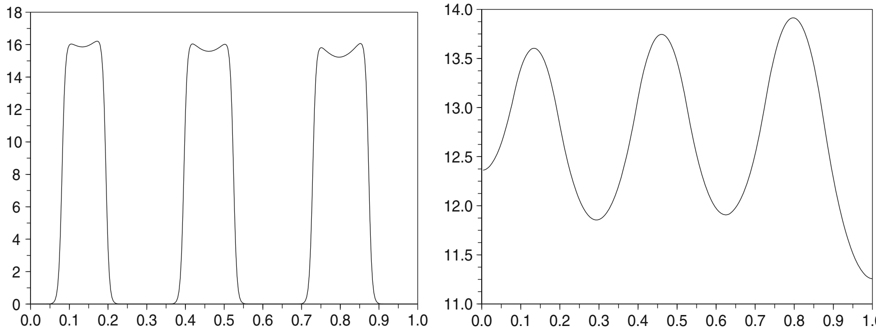

Fig. 7.7 The Turing patterns generated by the prey-predator system (7.34) with $\alpha = 1.8$, $\beta = 0.5$, $\gamma = 0.08$, $du = 0.001$ and $d_v = 0.6$. *Left*: component u, *Right*: component v. We have used 300 grid points for the computational domain $0 \le x \le 1$

Note also that the system has a priori bounds that follow from the maximum principle. If initially true, we have

$$\gamma \frac{u^2}{2} \le 1 + u \quad \Longrightarrow \quad u \le u_M := \frac{1 + \sqrt{1 - 2\gamma}}{\gamma},$$

$$v \le v_M := 1 + u_M.$$

Solution

1. The non-zero homogeneous steady state is given by $\bar{v} = \alpha\bar{u} + 1$ and

$$0 = \gamma \frac{\bar{u}^2}{2} - \bar{u} + \beta\bar{v} - 1 = \gamma \frac{\bar{u}^2}{2} + \bar{u}\,(\alpha\beta - 1) + \beta - 1.$$

Since $\beta < 1$, its positive solution is given by

$$\gamma\bar{u} = 1 - \alpha\beta + \sqrt{(1 - \alpha\beta)^2 + 2\gamma(1 - \beta)} > 2(1 - \alpha\beta).$$

2. The linearized matrix about this steady state is

$$A = \begin{pmatrix} \bar{u}(1 - \gamma\bar{u}) & -\beta\bar{u} \\ \\ \alpha\bar{v} & -\bar{v} \end{pmatrix}$$

3. We have $Tr(A) = \bar{u}(1 - \gamma\bar{u} - \alpha) - 1$ and $Tr(A) < 0$ if, and only if, $\bar{u}[1 - \alpha - \gamma\bar{u}] < 1$.
4. We have

$$Det(A) = -\bar{u}(1 - \gamma\bar{u})\bar{v} + \alpha\beta\bar{u}\bar{v} = \bar{u}\bar{v}\,(\alpha\beta + \gamma\bar{u} - 1)$$

and using question 1

$$Det(A) > \bar{u}\bar{v}\ (1 - \alpha\beta) > 0.$$

5. The last condition to have Turing instability is that one of the diagonal coefficients of A is positive. It can only be the upper left coefficient and this is satisfied if $\gamma\bar{u} < 1$.
6. As $\gamma \to 0$, we have $\gamma\bar{u} \to 2(1-\alpha\beta)$ and the condition $\alpha\beta < 1/2$ is sufficient to ensure $\gamma\bar{u} < 1$ for γ sufficiently small. We also have to ensure $\bar{u}[1-\alpha-\gamma\bar{u}] < 1$ (from question 3) and this converges to $\bar{u}[-1-\alpha+2\alpha\beta]$. in addition with $\alpha > 1$ we have in fact $[-1-\alpha+2\alpha\beta] < 0$, which guarantees the desired condition.
7. With these conditions we know from Theorem 7.1 that in a bounded domain, for d_u sufficiently small and d_v of the order of 1, the steady state is linearly unstable.

7.7 Keller-Segel with Growth

Exercise Consider the one dimensional Keller-Segel system with growth

$$\begin{cases} u_t - u_{xx} + \chi(uv_x)_x = u(1-u), & x \in \mathbb{R}, \\ -dv_{xx} + v = u. \end{cases} \tag{7.35}$$

1. Show that $u = 1$, $v = 1$ is a steady state.
2. Linearize the system around this steady state $(1, 1)$.
3. In the Fourier variable, reduce the system to a single equation for $\hat{U}(t, k)$,

$$\hat{U}_t + \hat{U}\ \Lambda(k) = 0,$$

and compute $\Lambda(k)$.
4. Show that it is linearly stable under the condition $\chi \le (1 + \sqrt{d})^2$.

Solution

1. This is easy.
2. $U_t - U_{xx} + \chi V_{xx} = -U, \qquad -dV_{xx} + V = U.$
3. $\hat{U}_t + k^2\hat{U} + k^2\chi\hat{V} = -\hat{U}, \qquad -dk^2\hat{V} + \hat{V} = \hat{U}.$
   We can eliminate $\hat{V}$ and find $\Lambda(k) = [k^2 + 1 - \chi\frac{k^2}{1+dk^2}]$.
4. The linear stability condition is that all solutions have the time decay $e^{-\lambda t}$ with $\lambda > 0$, in other words $\Lambda(k) > 0$. Using the shorter notation $X = k^2 \ge 0$, it reads $1 + X(d+1-\chi) + dX^2 \ge 0$. The analysis of the roots of this polynomial leads to 4.

References

1. Berestycki, H., Lions, P.-L.: Nonlinear scalar field equations, II. Existence of infinitely many solutions. Arch. Ration. Mech. Anal. **82**(4), 347–375 (1983)
2. Berestycki, H., Nicolaenko, B., Scheurer, B.: Traveling wave solutions to combustion models and their singular limits. SIAM J. Math. Anal. **16**(6), 1207–1242 (1985)
3. Berestycki, H., Nadin, G., Perthame, B., Ryzhik, L.: The non-local Fisher-KPP equation: traveling waves and steady states. Nonlinearity **22**, 2813–2844 (2009)
4. Britton, N.F.: Spatial structures and periodic traveling waves in an integro-differential reaction-diffusion population model. SIAM J. Appl. Math. **50**(6), 1663–1688 (1990)
5. Castets, V., Dulos, E., Boissonade, J., De Kepper, P.: Experimental evidence of a sustained standing Turing-type nonequilibrium chemical pattern. Phys. Rev. Lett. **64**(24), 2953–2956 (1990)
6. De Kepper, P., Castets, V., Dulos, E., Boissonade, J.: Turing-type chemical patterns in the chlorite-iodide-malonic acid reaction. Physica D **49**, 161–169 (1991)
7. FreeFEM++: Software available at http://www.freefem.org (2015)
8. Génieys, S., Volpert, V., Auger, P.: Pattern and waves for a model in population dynamic with non-local consumption of resources. Math. Model. Nat. Phenom. **1**(1), 65–82 (2006)
9. Gierer, A., Meinhardt, H.: A theory of biological pattern formation. Kybernetik **12**, 30–39 (1972)
10. Gourley, S.A.: Travelling front solutions of a non-local Fisher equation. J. Math. Biol. **41**, 272–284 (2000)
11. Gray, P., Scott, S.K.: Autocatalytic reactions in the isothermal continuous stirred tank reactor: isolas and other forms of multistability. Chem. Eng. Sci. **38**(1), 29–43 (1983)
12. Hecht, F.: New development in FreeFEM++. J. Numer. Math. **20**(3–4), 251–265 (2012)
13. Kolokolnikov, T., Ward, M.J., Wei, J.: Spot self-replication and dynamic for the Schnakenburg model in a two-dimensional domain. J. Nonlinear Sci. **19**(1), 1–56 (2009)
14. Kondo, S., Asai, R.: A reaction-diffusion wave on the skin of the marine angelfish *Pomacanthus*. Nature **376**, 765–768 (1995)
15. Lefever, R., Lejeune, O.: On the origin of tiger bush. Bull. Math. Biol. **59**(2), 263–294 (1997)
16. Lengyel, I., Epstein, I.R.: Modeling of Turing structure in the chlorite-iodide-malonic acid-starch reaction system. Science **251**, 650–652 (1991)
17. Logak, E., Loubeau, V.: Travelling wave solutions to a condensed phase combustion model. Asymptot. Anal. **12**(4), 259–294 (1996)
18. Maini, P.K.: How the mouse got its stripes. PNAS **100**(17), 9656–9657 (2003). doi:10.1073/pnas.1734061100
19. Malchiodi, A., Montenegro, M.: Multidimensional boundary layers for a singularly perturbed Neumann problem. Duke Math. J. **124**, 105–143 (2004)
20. Marion, M.: Qualitative properties of a nonlinear system for laminar flames without ignition temperature. Nonlinear Anal. **9**(11), 1269–1292 (1985)
21. Meinhardt, H.: Models of Biological Pattern Formation. Academic, London (1982)
22. Meinhardt, H.: The Algorithmic Beauty of Sea Shells. Springer, Heidelberg (1995)
23. Morita, Y., Ogawa, T.: Stability and bifurcation of nonconstant solutions of a reaction-diffusion system with conservation of mass. Nonlinearity **23**, 1387–1411 (2010)
24. Muratov, C.B., Osipov, V.V.: Traveling spike autosolitons in the Gray-Scott model. Physica D **155**, 112–131 (2001)
25. Murray, J.D.: Mathematical Biology, vols. 1 and 2, 2nd edn. Springer, New York (2002)
26. Nadin, G., Perthame, B., Tang, M.: Can a traveling wave connect two unstable states? The case of the nonlocal Fisher equation. C. R. Acad. Sci. Paris Ser. I **349**, 553–557 (2011)
27. Ni, W., Tang, M.: Turing patterns in the Lengyel-Epstein system for the CIMA reaction. Trans. Am. Math. Soc. **357**, 3953–3969 (2005)
28. Ni, W.-M., Wei, J.: On positive solutions concentrating on spheres for the Gierer–Meinhardt system. J. Diff. Equ. **221**, 158–189 (2006)

29. Nicolis, G., Prigogine, I.: Self-organization in Non-equilibrium Systems. Wiley Interscience, New-York (1977)
30. Oster, G.F., Shubin, N., Murray, J.D., Alberch, P.: Evolution and morphogenetic rules: the shape of the vertebrate limb in ontogeny and phylogeny. Evolution **45**, 862–884 (1988)
31. Prigogine, I., Lefever, R.: Symmetry breaking instabilities in dissipative systems, II. J. Chem. Phys. **48**, 1695–1700 (1968)
32. Schnakenberg, J., Simple chemical reactions with limit cycle behavior. J. Theor. Biol. **81**, 389–400 (1979)
33. Turing, A.M.: The chemical basis of morphogenesis. Philos. Trans. R. Soc. B **237**, 37–72 (1952)
34. Wei, J., Winter, M.: Symmetric and asymmetric multiple clusters in a reaction-diffusion system. NoDEA **14**(5–6), 787–823 (2007)
35. Yi, F., Wei, J., Shi, J.: Diffusion-driven instability and bifurcation in the Lengyel-Epstein reaction-diffusion system. Nonlinear Anal. Real World Appl. **9**, 1038–1051 (2008)

Chapter 8
The Fokker-Planck Equation

Not only diffusion but also drift terms (first order derivatives) are used in order to describe motion when a velocity field is applied. We begin with a particular Fokker-Planck equation where the drift is the gradient of a given smooth potential $V : \mathbb{R}^d \to \mathbb{R}$

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \Delta n(t,x) - \operatorname{div}\big(n(t,x)\nabla V(x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.1}$$

There are many interpretations, applications and derivations from biology that motivate the use of this equation. Just to mention some of them

- Active motion with the velocity $U = -\nabla V(x)$ in addition to Brownian motion (see Sects. 8.4 and 8.6). For this reason, in nonlinear contexts, Eq. (8.1) is often called the *drift-diffusion equation*.
- Noise, and this appears in many models of neuroscience.
- Chemistry as an intermediate model between the molecular level and reaction rate equations when they cannot be applied, see Sect. 1.2 and in particular, Sect. 1.2.6.
- Asymptotic limits in various formulations. Examples are scattering of waves or jump processes (see Chap. 9).
- More generally, the Fokker-Planck equation describes the probability density of stochastic differential equations. For this reason, Eq. (8.1) is also called the *Kolmogorov equation* and can appear in any dimension with very general forms.

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_8

8.1 Elementary A Priori Estimates

The main properties of solutions of (8.1) are the nonnegativity principle, the 'mass' conservation and the existence of a non-zero steady state,

$$n^0 \geq 0 \implies n(t,x) \geq 0, \tag{8.2}$$

$$\int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} n^0(x)dx, \quad \forall t \geq 0, \tag{8.3}$$

$$\mu e^{-V(x)} \qquad \text{are steady states for all } \mu \in \mathbb{R}, \tag{8.4}$$

this last statement is because $\Delta e^{-V} = \operatorname{div}(\nabla e^{-V}) = -\operatorname{div}(e^{-V}\nabla V)$.

It is intuitive that the decay properties of this steady state should play a role, for example because its integrability is a desirable property. This relies on growth assumptions of $V(x)$ at infinity. A potential V is called *confining* if $V(x) \to +\infty$ as $|x| \to \infty$; typically $V(x) = \frac{|x|^2}{2}$ determines a Gaussian steady state.

A simple idea is to look directly for a priori estimates in L^2. After multiplication by n and integration by parts, one finds

$$\begin{aligned} \tfrac{1}{2}\tfrac{d}{dt}\textstyle\int_{\mathbb{R}^d} n(t,x)^2dx + \int_{\mathbb{R}^d} |\nabla n(t,x)|^2dx &= -\textstyle\int_{\mathbb{R}^d} \nabla n(t,x)\ \nabla V(x)n(t,x)dx \\ &= -\tfrac{1}{2}\textstyle\int_{\mathbb{R}^d} \nabla n(t,x)^2\ \nabla V(x)dx \end{aligned}$$

and thus we arrive at

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} n(t,x)^2dx + \int_{\mathbb{R}^d} |\nabla n(t,x)|^2dx = \frac{1}{2}\int_{\mathbb{R}^d} n(t,x)^2\ \Delta V(x)dx. \tag{8.5}$$

When $\Delta V \leq -\nu < 0$, with ν a constant, one finds that

$$\int_{\mathbb{R}^d} n(t,x)^2dx \leq e^{-\nu t}\int_{\mathbb{R}^d} n^0(x)^2dx.$$

Note that, in this case, the steady state in (8.4) is not integrable and this calculation shows the interest of confining potentials.

8.2 The Relative Entropy

Additional to (8.2), (8.3) and (8.5), there is another family of notable a priori estimates for solutions of (8.1), the so-called *relative entropy* inequalities. They improve the L^2 inequality in the sense that they do not require any derivative of the potential

Proposition 8.1 *For any convex function $H : \mathbb{R} \to \mathbb{R}$, we have*

$$\frac{d}{dt}\int_{\mathbb{R}^d} e^{-V(x)} H\left(\frac{n(t,x)}{e^{-V(x)}}\right) dx = -D_H(n|e^{-V}) \le 0,$$

$$D_H(n|e^{-V}) := \int_{\mathbb{R}^d} e^{-V} H''\left(\frac{n}{e^{-V}}\right) \left|\nabla \frac{n}{e^{-V}}\right|^2 dx.$$

We postpone the proof after some comments.

A special case is $V = 0$, then we simply find the usual heat equation and the usual L^p estimates when choosing $H(u) = u^p$. In general, the L^p estimates are true but they come with weights. More precisely, we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^d} e^{(p-1)V(x)} n^p(t,x) dx \le 0.$$

With $H(u) = u \ln(u)$, one finds the inequality

$$\frac{d}{dt}\int_{\mathbb{R}^d} [n(t,x)\ln n(t,x) + n(t,x)V(x)]dx \le 0.$$

From the proof, we also derive, in the same way, the comparison principle

Corollary 8.2 *For a subsolution $\underline{n}$, that is,*

$$\begin{cases} \frac{\partial}{\partial t}\underline{n} - \Delta \underline{n} - \operatorname{div}\big(\underline{n}\nabla V\big) \le 0, & t \ge 0,\ x \in \mathbb{R}^d, \\ \underline{n}(t=0,x) \le n^0(x), \end{cases} \tag{8.6}$$

we have $\underline{n} \le n$.

Proof of Corollary 8.2 Re-do the proof of the relative entropy inequality in Proposition 8.1 for subsolutions, with the properties that H is convex *and non-decreasing*, and prove that the entropy relation holds as an inequality

$$\frac{d}{dt}\int_{\mathbb{R}^d} e^{-V(x)} H\left(\frac{\underline{n}(t,x)}{e^{-V(x)}}\right) dx \le -D_H(\underline{n}|e^{-V}) \le 0.$$

Apply it to $\underline{n} - n$ with $H(u) = (u)_+$, which initially will vanish and thus vanishes for all times. □

Another consequence of the relative entropy inequality is the maximum principle

Corollary 8.3 *If, for some constant $C^0_\pm$, we have $-C^0_- e^{-V} \le n^0 \le C^0_+ e^{-V}$ then*

$$-C^0_- e^{-V} \le n(t,\cdot) \le C^0_+ e^{-V}, \qquad \forall t \ge 0.$$

The case $C^0_- = 0$ gives the positivity principle mentioned in the introduction.

Proof of Corollary 8.3 The proof is a variant of the method of Stampacchia. We choose the convex function $H(u) = \big(u - C_+^0\big)_+^2$ so that, at initial time

$$e^{-V(x)} H\left(\frac{n^0(x)}{e^{-V(x)}}\right) = 0.$$

Consequently, the relative entropy inequality in Proposition 8.1 shows that for all $t \geq 0$,

$$\int_{\mathbb{R}^d} e^{-V(x)} H\left(\frac{n(t,x)}{e^{-V(x)}}\right) dx \leq 0,$$

and because $H(\cdot) \geq 0$, this means that $\frac{n(t,x)}{e^{-V(x)}} \leq C_+^0$ and the upper bound is proved. The lower bound is proved in a similar way. □

Proof of Proposition 8.1 One can write the Fokker-Planck equation (8.1) as

$$\frac{\partial}{\partial t} n(t,x) - \text{div}\big[e^{-V(x)} \nabla \big(n\, e^{V(x)}\big)\big] = 0,$$

and $u = n\, e^{V(x)}$ satisfies

$$\frac{\partial}{\partial t}[u e^{-V}] - \text{div}\big[e^{-V(x)} \nabla u\big] = 0,$$

or the 'strong form'

$$\frac{\partial}{\partial t} u - \Delta u + \nabla V . \nabla u = 0.$$

From this, we conclude that for any (sufficiently smooth) convex function $H : \mathbb{R} \to \mathbb{R}$, we have

$$\frac{\partial}{\partial t} H(u) - \Delta H(u) + \nabla V . \nabla H(u) = -H''(u) |\nabla u|^2.$$

Or going back to a conservative form

$$\frac{\partial}{\partial t}[H(u) e^{-V}] - \text{div}\big[e^{-V} \nabla H(u)\big] = -H''(u) e^{-V} |\nabla u|^2.$$

The result follows integrating in x. □

Exercise

1. Prove that for two solutions $n_1, n_2 > 0$ (with different initial data), one also has

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_2(t,x) H\left(\frac{n_1(t,x)}{n_2(t,x)}\right) dx \le 0.$$

2. Use this to prove that for $n(t,x) > 0$ and $H(\cdot)$ convex, we have

$$\frac{d}{dt}\int_{\mathbb{R}^d} n(t,x) H\left(\frac{\partial \ln\big(n(t,x)\big)}{\partial t}\right) dx \le 0.$$

3. Conclude that $\max_{x\in\mathbb{R}^d} \frac{\partial \ln\big(n(t,x)\big)}{\partial t}$ decreases.

8.3 Weak Solutions

As we did in Chap. 3, we define a weak solution of (8.1) by testing against functions $\Phi \in \mathcal{D}(\mathbb{R}^+ \times \mathbb{R}^d)$

$$\int_0^\infty \int_{\mathbb{R}^d} n(t,x)\left[-\frac{\partial \Phi}{\partial t} - \Delta\Phi + \nabla V.\nabla\Phi\right] dx\, dt = \int_{\mathbb{R}^d} n^0(x)\Phi(0,x)dx. \tag{8.7}$$

We see that this makes sense under different assumptions for V. Examples are

- assume $\nabla V \in L^2_{loc}(\mathbb{R}^d)$ and $n \in L^\infty\big((0,T); L^2(\mathbb{R}^d)\big)$ for all $T > 0$,
- assume $\nabla V \in C(\mathbb{R}^d)$ and $n \in L^\infty\big(\mathbb{R}^+; M^1(\mathbb{R}^d)\big)$ (bounded measure), which is relevant in view of mass conservation.

Another option is to use, as we did for the relative entropy structure, the alternative formulation

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \operatorname{div}\big(e^{-V(x)}\nabla(n(t,x)e^{V(x)})\big) = 0, & t \ge 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.8}$$

This leads to another possible weak formulation

$$\int_0^\infty \int_{\mathbb{R}^d} n(t,x)\left[-\frac{\partial \Phi}{\partial t} - e^{V(x)}\operatorname{div}\big(e^{-V(x)}\nabla\Phi\big)\right] dx\, dt = \int_{\mathbb{R}^d} n^0(x)\Phi(0,x)dx,$$

which is not very different from (8.7).

When applying the Lax-Milgram theory [2, 6, 7] for steady states, the two formulations are however very different. The direct formulation leads to the use of the scalar product (definiteness should come from the zero order term for example)

$$((n,\Phi))_1 = \int_{\mathbb{R}^d} \nabla n(x).\nabla\Phi(x)dx + \int_{\mathbb{R}^d} n(x)\nabla\Phi(x).\nabla V dx.$$

The modified formulation leads to the scalar product (we use the test function $\Phi(x) = \phi(x)e^{V(x)}$)

$$((n,\phi))_2 = \int_{\mathbb{R}^d} \nabla(n(x)e^{V(x)}).\nabla(\phi(x)e^{V(x)})e^{-V(x)}dx = \int_{\mathbb{R}^d} \nabla\tilde{n}(x).\nabla\Phi(x)e^{-V(x)}dx.$$

This is a self-adjoint scalar product in the Hilbert space $H^1(e^{-V(x)}dx)$, with definiteness directly related to the Poincaré inequality in the full space. See Ledoux [11].

8.4 The Deterministic Case

The case without diffusion makes sense and is called the *transport equation*. These equations belong to the class of hyperbolic equations and it is useful to first consider the strong form

The Strong Form This refers to the equation

$$\begin{cases} -\frac{\partial}{\partial t}u(t,x) - U(t,x).\nabla u = 0, & t \ge 0,\ x \in \mathbb{R}^d, \\ u(t=0,x) = u^0(x) \in C^1(\mathbb{R}^d). \end{cases} \tag{8.9}$$

When U is a Lipschitz continuous vector field $\mathbb{R}\times\mathbb{R}^d \to \mathbb{R}^d$, it can be solved using the *method of characteristics*.

Definition 8.4 The characteristics are the solutions of the Ordinary Differential System

$$\begin{cases} \frac{dX(t;x^0)}{dt} = U(t, X(t;x^0)), \\ X(0) = x^0 \in \mathbb{R}^d. \end{cases} \tag{8.10}$$

Lemma 8.5 *The solution of* (8.9) *is given thanks to the formula*

$$u(t, X(t;x^0)) = u^0(x^0) \qquad \forall t \ge 0,\ \forall x^0 \in \mathbb{R}^d.$$

In other words, solutions are constant along the characteristics.

Proof For a C^1 function one can write

$$\begin{aligned}\tfrac{d}{dt}u(t, X(t; x^0)) &= \tfrac{\partial}{\partial t}u(t, X(t; x^0)) + \dot{X}(t; x^0).\nabla u(t, X(t; x^0))\\ &= \tfrac{\partial}{\partial t}u(t, X(t; x^0)) + U\big(X(t; x^0)\big).\nabla u(t, X(t; x^0)).\end{aligned}$$

This derivative vanishes if, and only if, the transport equation (8.9) is satisfied. Note that the Cauchy-Lipschitz theorem tells us that, when x^0 cover $\mathbb{R}^d$, then $X(t; x^0)$ also covers $\mathbb{R}^d$. □

The Divergence (Conservative) Form This is the Fokker-Planck equation where we neglect diffusion,

$$\begin{cases} \tfrac{\partial}{\partial t}n(t, x) + \operatorname{div}\big(n(t, x)U(t, x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ n(t = 0, x) = n^0(x). \end{cases} \tag{8.11}$$

A first result, which gives a simple representation formula for the solution is

Lemma 8.6 *For* $n^0(x) := \sum_{k=1}^{K} \rho_k^0 \delta(x - x_k^0)$*, the solution of* (8.11) *is given by the formula*

$$n(t, x) = \sum_{k=1}^{K} \rho_k^0 \delta\big(x - X(t; x_k^0)\big).$$

More generally, we may represent the initial data as $n^0(x) = \int_{\mathbb{R}^d} n^0(y)\delta(x - y)$ (replacing the finite sum by an integral) and we find

$$n(t, x) = \int_{\mathbb{R}^d} n^0(y)\delta\big(x - X(t; y)\big)dy. \tag{8.12}$$

For this reason we see that the population density is transported by the flow field U. We also see that L^1 is a relevant space for $n^0 \in L^1$ by mass conservation $\int_{\mathbb{R}^d} n(t, x)dx = \int_{\mathbb{R}^d} n^0(x)dx$.

Proof of Lemma 8.6 Because this is a linear equation, we only have to prove the formula for one Dirac mass and the weight $\rho^0 = 1$. Then, the definition of a weak solution means that for all smooth test functions $u(t, x)$ we have, for all $T > 0$,

$$\int_{\mathbb{R}^d} n(T, x)u(T, x) - \int_0^T \int_{\mathbb{R}^d} n(t, x)\big[\frac{\partial}{\partial t}u(t, x) + U(t, x).\nabla u(t, x)\big] = \int_{\mathbb{R}^d} u\big(0, x\big).$$

For the Dirac mass this is to say

$$u(T,X(T;x^0))-\int_0^T \big[\frac{\partial}{\partial t}u(t,X(t;x^0))+U(t,X(t;x^0)).\nabla u(t,X(t;x^0))\big] = \int_{\mathbb{R}^d} u\big(0,x^0\big)$$

arguing as in the proof of Lemma 8.5, we remark that

$$\frac{\partial}{\partial t}u(t,X(t;x^0)) + U(t,X(t;x^0)).\nabla u(t,X(t;x^0)) = \frac{d}{dt}u(t,X(t;x^0))$$

and the result follows. □

Despite the simple form for the Dirac initial data, the general formula for the solution of Eq. (8.11) is not simple and can be derived from the expression

$$\frac{\partial}{\partial t}n(t,x) + U(t,x).\nabla n(t,x) + n(t,x)\mathrm{div}U = 0.$$

Using the proof of Lemma 8.5 one finds

$$n(t,X(t,y)) \ \exp \int_0^t \mathrm{div}U\,(s,X(s;y)ds = n^0(y) \qquad \forall t \geq 0,\ \forall y \in \mathbb{R}^d. \tag{8.13}$$

This expression is not very convenient but one readily checks again that

$$n^0 \geq 0 \implies n(t,x) \geq 0, \qquad \int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} n^0(x)dx.$$

8.5 The Complete Fokker-Planck Equation

The complete Fokker-Planck equation (also called the Kolmogorov equation in the theory of Markov/diffusion processes) is given by

$$\begin{cases} \frac{\partial}{\partial t}n(t,x) - \frac{1}{2}\sum_{i,j=1}^{d}\frac{\partial^2}{\partial x_i\,\partial x_j}\big(B_{ij}(t,x)n(t,x)\big) + \mathrm{div}\big(n(t,x)U(t,x)\big) = 0, \quad t \geq 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.14}$$

Here $U : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$ is the velocity field and $B : \mathbb{R}^+ \times \mathbb{R}^d \to \mathcal{M}_+^{d\times d}$ is the nonnegative symmetric diffusion matrix. In other words, it is always assumed to satisfy, for some constant $\nu \geq 0$,

$$\sum_{i,j=1}^{d} B_{ij}(t,x)\xi_i\xi_j \geq \nu|\xi|^2 \qquad \forall \xi \in \mathbb{R}^d.$$

The main properties are still the sign property

$$n^0 \geq 0 \implies n \geq 0,$$

and 'mass' conservation

$$\int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} n^0(x)dx, \quad \forall t \geq 0.$$

We assume that there is a steady state $N(x)$ to (8.1)

$$-\frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \, \partial x_j}\big(B_{ij}(x)N(x)\big) + \operatorname{div}\big(N(x)U(x)\big) = 0, \quad \forall x \in \mathbb{R}^d, \qquad N(x) > 0. \tag{8.15}$$

The existence of solutions depends heavily on the coefficients (B, U) and on the desired properties for N (usually $N \in L^1 \cap L^\infty(\mathbb{R}^d)$), but a typical example is as before

$$\frac{1}{2}B = I \quad \text{(identity matrix)}, \qquad U(x) = -\nabla V(x), \qquad N(x) = \mu e^{-V(x)}, \; \mu \in \mathbb{R}.$$

More generally for a constant matrix B, when $U = -B\nabla V(x)$, we find the same steady states.

For this general equation, we still have the relative entropy relation

Proposition 8.7 *For any convex function $H : \mathbb{R} \to \mathbb{R}$, we have*

$$\frac{d}{dt}\int_{\mathbb{R}^d} N(x)H\left(\frac{n(t,x)}{N(x)}\right)dx = -D_H(n|N) \leq 0,$$

$$D_H(n|N) = \frac{1}{2}\sum_{i,j=1}^{d}\int_{\mathbb{R}^d} N(x)B_{ij}(x)\nabla_{x_i}\left(\frac{n}{N}\right)\,\nabla_{x_j}\left(\frac{n}{N}\right)dx.$$

To prove it, calculate successively the equation for $u(t,x) = \frac{n(t,x)}{N(x)}$, then for $H\big(u(t,x)\big)$, and then for $NH\big(u(t,x)\big)$. It is tedious but it works.

There are many examples of nonlinear Fokker-Planck equations arising in biology and we give examples later. They describe the density of a population moving with a deterministic velocity U added to a 'random noise of intensity' a_{ij}. More generally, the reason why Fokker-Planck equations play a central role is the connection with Brownian motion and Stochastic Differential Equations. This material is introduced below.

8.6 Stochastic Differential Equations (SDE)

The Fokker-Planck equation is intimately connected to Stochastic Differential Equations and we explain this in the next three sections. As we did in Sect. 1.4 for Brownian motion, we give here a very intuitive and non-rigorous construction based on numerical approximations. For a given, sufficiently smooth, vector field $U \in \mathbb{R}^d$ and a matrix $\sigma(t,x) \in M_{d,p}$, one can build the solution of the Itō Stochastic Differential Equation (see Fig. 8.1)

$$\begin{cases} dX(t) = U\big(t, X(t)\big)dt + \sigma\big(t, X(t)\big)dW(t), \\ X(0) = X^0 \in \mathbb{R}^d \quad \text{(a random vector)}, \end{cases} \tag{8.16}$$

with $W(t) = \big(W^1(t), \dots W^p(t)\big)$, p independent Brownian motions.

The numerical construction mimics the one in Sect. 1.4 and we use the same notations. This defines the Euler scheme (here we calculate with $d = p = 1$ but the reader can extend it easily)

$$X^{k+1} = X^k + \Delta t\, U\big(t^k, X^k\big) + \sqrt{\Delta t}\, \sigma\big(t^k, X^k\big) Y^k. \tag{8.17}$$

Because the random variable Y^k is independent of X^k and $\mathbb{E}[Y^k] = 0$, we have

$$\mathbb{E}\left[X^{k+1} - X^k\right] = \Delta t \mathbb{E}\big[U\big(t^k, X^k\big)\big], \tag{8.18}$$

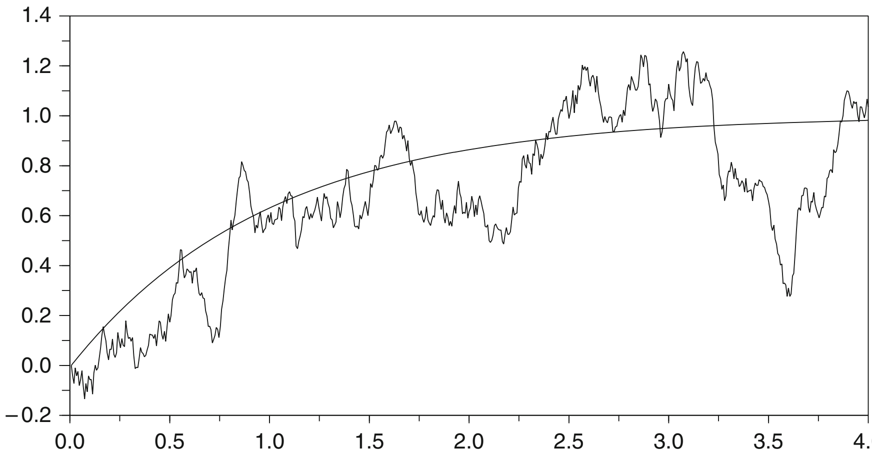

Fig. 8.1 Deterministic solution ($\sigma = 0$) and a path solution ($\sigma = \frac{1}{2}$) to the Itō SDE (8.17) for the drift $U(x) = 1 - x$

$$\begin{aligned}\mathbb{E}\left[\left(X^{k+1}-X^k\right)^2\right] &= \mathbb{E}\left[\Delta t^2 U^2\left(t^k,X^k\right)+2\Delta t^{3/2}U\left(t^k,X^k\right)\sigma\left(t^k,X^k\right)Y^k\right.\\ &\qquad \left.+\Delta t\left|\sigma\left(t^k,X^k\right)Y^k\right|^2\right]\\ &= \Delta t\ \mathbb{E}\left[\sigma^2\left(t^k,X^k\right)\right]\mathbb{E}\left[\left(Y^k\right)^2\right]+O(\Delta t^2)\\ &= \Delta t\ \mathbb{E}\left[\sigma^2\left(t^k,X^k\right)\right]+O(\Delta t^2).\end{aligned}$$

Except when $\sigma \equiv 0$, this scales like the Brownian motion.

The type of approximation scheme used in (8.17) is very important, in opposition to the deterministic case. Changing this approximation also changes the limit. The Stratonovich convention is an example and the notion is denoted as

$$\begin{cases} dX(t) = U\big(t,X(t)\big)dt + \sigma\big(t,X(t)\big)\circ dW(t), \\ X(0) = X^0 \in \mathbb{R}^d \quad \text{(a random vector).} \end{cases} \tag{8.19}$$

The Stratonovich SDE corresponds to the semi-implicit approximation in the stochastic term

$$X^{k+1} = X^k + \Delta t\ U\big(t^k,X^k\big) + \sqrt{\Delta t}\,\sigma\big(t^k,\frac{X^k+X^{k+1}}{2}\big)Y^k. \tag{8.20}$$

It may be may approximated as

$$\begin{aligned}X^{k+1} &\approx X^k + \Delta t\ U\big(t^k,X^k\big) + \sqrt{\Delta t}\left[\sigma\big(t^k,X^k\big)+\tfrac{1}{2}D\sigma\big(t^k,X^k\big)(X^{k+1}-X^k)\right]Y^k\\ &\approx X^k + \Delta t\ U\big(t^k,X^k\big) + \tfrac{\Delta t}{2}D\sigma\big(t^k,X^k\big)\sigma\big(t,X^k\big)\big(Y^k\big)^2\\ &\quad +\sqrt{\Delta t}\,\sigma\big(t^k,X^k\big)Y^k + O(\Delta t^{3/2}).\end{aligned}$$

This means that

$$\mathbb{E}\left[X^{k+1}-X^k\right] = \Delta t\mathbb{E}\left[U\big(t^k,X^k\big)\right] + \frac{\Delta t}{2}\mathbb{E}\left[D\sigma\big(t^k,X^k\big)\sigma\big(t^k,X^k\big)\big)\right], \tag{8.21}$$

in other words, one cannot take the expectation as simply as for Itō SDE.

Because $\mathbb{E}\left[(Y^k)^3\right] = 0$, we also find that

$$\mathbb{E}\left[\left(X^{k+1}-X^k\right)^2\right] = \Delta t\ \mathbb{E}\left[\sigma^2\left(t^k,X^k\right)\right]+O(\Delta t^2).$$

It is remarkable that the Stratonovich semi-implicit scheme leads to the same first two expectations as the Itō formula with the drift U changed in $U - \frac{1}{2}\sigma'\sigma$; in fact for the limit $\Delta t \to 0$, the two constructions are equivalent with this modification for the drift. This is to say that the limit of the term $\big(Y^k\big)^2$ is 1 in probability.

8.7 The Itō Formula

An important tool in the theory of SDEs is the Itō formula that gives the equation satisfied by the random variable $u(t, X(t))$, when $u \in C^2(\mathbb{R}^{d+1}; \mathbb{R})$,

$$du(t, X(t)) = \Big[\tfrac{\partial u(t,X(t))}{\partial t} + U\big(t, X(t)\big).Du\big(t, X(t)\big) + \tfrac{1}{2}B\big(t, X(t)\big).D^2u\big(t, X(t)\big)\Big]\, dt$$
$$+\sigma\big(t, X(t)\big).Du\big(t, X(t)\big).dW(t) \tag{8.22}$$

with

$$B(t, x) = \frac{1}{2}\sigma(t, x).\sigma^t(t, x) \qquad (\sigma^t \text{ denotes the transposed matrix}). \tag{8.23}$$

In other words, the chain rule does not apply to SDEs as it applies to ODEs ($\sigma(t, x) = 0$) and it gives an additional term, namely the term $B\big(t, X(t)\big).D^2u\big(t, X(t)\big)$.

This formula can be derived from the approximation (8.17). Using Taylor's expansion in time, we find (again with $d = p = 1$ to simplify)

$$\begin{aligned} u(t^{k+1}, X^{k+1}) &= u(t^k, X^{k+1}) + \Delta t\tfrac{\partial u(t^k,X^{k+1})}{\partial t} + O(\Delta t^2) \\ &= u(t^k, X^{k+1}) + \Delta t\tfrac{\partial u(t^k,X^k)}{\partial t} + O(\Delta t^{3/2}). \end{aligned}$$

Therefore, using now Taylor's expansion in space, we find

$$\begin{aligned} u(t^{k+1}, X^{k+1}) = u(t^k, X^k) &+ \Delta t\tfrac{\partial u(t^k,X^k)}{\partial t} + O(\Delta t^{3/2}) \\ &+\big[\Delta t U(t^k, X^k) + \sqrt{\Delta t}\,\sigma\big(t^k, X^k\big)Y^k\big].Du(t^k, X^k) \\ &+\tfrac{1}{2}\Delta t\sigma^2\big(t^k, X^k\big)\big(Y^k\big)^2 D^2u(t^k, X^k). \end{aligned}$$

As we already saw for the Stratonovich model, the limit of the term $\big(Y^k\big)^2$ is 1 for the limit $\Delta t \to 0$ and we see that this is the discrete version of (8.22).

In the case of the Stratonovich convention, one can use the chain rule as in the deterministic case (and this is the advantage gained from the more complicated average)

$$du(t, X(t)) = \left[\frac{\partial u(t, X(t))}{\partial t} + U\big(t, X(t)\big).Du\big(t, X(t)\big)\right]\Delta t$$
$$+\sigma\big(t, X(t)\big).Du\big(t, X(t)\big) \circ dW(t). \tag{8.24}$$

To see this, we can redo the discrete version, and to simplify, use a function of X only,

$$u(X^{k+1}) = u(X^k) + Du(X^k)[\Delta t\ U\big(t^k, X^k\big) + \sqrt{\Delta t}\,\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)Y^k]$$
$$+\tfrac{\Delta t}{2}D^2u(X^k)\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)^2(Y^k)^2 + O(\Delta t^{3/2}),$$

which we may 'center' to follow the semi-implicit rule

$$u(X^{k+1}) = u(X^k) + \Delta t\ Du(X^k)U\big(t^k, X^k\big) + \sqrt{\Delta t}\ Du\big(\tfrac{X^k+X^{k+1}}{2}\big)\sqrt{\Delta t}\,\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)Y^k$$
$$-\tfrac{\sqrt{\Delta t}}{2}D^2u(X^k)(X^{k+1}-X^k)\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)^2Y^k$$
$$+\tfrac{\Delta t}{2}D^2u(X^k)\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)^2(Y^k)^2 + O(\Delta t^{3/2})$$

and because the dominant term in $X^{k+1} - X^k$ is $\sqrt{\Delta t}\,\sigma\big(\frac{X^k+X^{k+1}}{2}\big)Y^k$, we finally end up with

$$u(X^{k+1}) = u(X^k) + \Delta t\ Du(X^k)U\big(t^k, X^k\big)$$
$$+\sqrt{\Delta t}\ Du\Big(\frac{X^k+X^{k+1}}{2}\Big)\sigma\Big(\frac{X^k+X^{k+1}}{2}\Big)Y^k + O(\Delta t^{3/2}),$$

which is the discrete version of (8.24).

8.8 The Kolmogorov Equation

To go further and make the link with the Fokker-Planck equation, we recall the

Definition 8.8 The probability density $n(x)$ of a random variable X is defined by the identity

$$\int u(x)n(x)dx = \mathbb{E}\big[u(X(\omega))\big],$$

for all smooth test functions u with compact support.

We give the probability density $n^0(x)$ of X^0 and we denote by $n(t,x)$ the probability density of the process $X(t,\omega)$. Then, we can deduce from the Itō formula that

Theorem 8.9 (Fokker-Planck-Kolmogorov Equation) *For the process* (8.17)*, the limiting probability density* $n(t,x)$ *satisfies the Fokker-Planck equation* (8.14)*.*

Remark that the construction of $n(t,x)$ gives the 'mass conservation' property because, for a probability density, we have $\int_{\mathbb{R}^d} n(t,x)dx = 1$. We give two derivations of this fact.

Proof We give two derivations. To see this from the SDE, we write, taking the expectation in (8.22), that for any smooth function $u(t,x)$, we have

$$\frac{d}{dt}\mathbb{E}\big[u(t,X(t)\big] = \mathbb{E}\bigg[\frac{\partial u(t,X(t))}{\partial t} + U\big(t,X(t)\big).Du\big(t,X(t)\big)$$
$$+\frac{1}{2}B\big(t,X(t)\big).D^2u\big(t,X(t)\big)\bigg].$$

Using the definition of the probability density $n(t,x)$ of the process $X(t)$, the former identity is also written

$$\frac{d}{dt}\int u(t,x)n(t,x)dx = \int \frac{\partial u(t,x)}{\partial t}n(t,x)dx$$
$$+\int \big[U(t,x).Du(t,x) + \frac{1}{2}B(t,x).D^2u(t,x)\big]n(t,x)dx.$$

The chain rule gives

$$\frac{d}{dt}\int u(t,x)n(t,x)dx = \int \frac{\partial u(t,x)}{\partial t}n(t,x)dx + \int u(t,x)\frac{\partial n(t,x)}{\partial t}dx,$$

and thus we find

$$0 = -\int u(t,x)\frac{\partial n(t,x)}{\partial t}dx + \int \big[U(t,x).Du(t,x) + \frac{1}{2}B(t,x).D^2u(t,x)\big]n(t,x)dx,$$

and after integration by parts

$$0 = \int u(t,x)\bigg[-\frac{\partial n(t,x)}{\partial t} - \mathrm{div}[U(t,x).n(t,x)] + D^2[\frac{1}{2}B(t,x).n(t,x)]\bigg]dx.$$

This holds true for any test function $u(t,x)$, therefore we conclude that

$$-\frac{\partial n(t,x)}{\partial t} - \mathrm{div}[U(t,x).n(t,x)] + D^2[\frac{1}{2}B(t,x).n(t,x)] = 0,$$

that is, the complete Fokker-Planck equation (8.14).

We can give another derivation based on the Euler discrete scheme (8.17) and write for all smooth functions $u(x)$ that, still with N the normal law, we have

$$u(X^{k+1}) = u\Big(X^k + \Delta t\, U\big(t^k,X^k\big) + \sqrt{\Delta t}\,\sigma\big(t^k,X^k\big)Y^k\Big),$$

$$\int u(x)n^{k+1}(x)dx = \int\int u\Big(x + \Delta t U(t^k,x) + \sqrt{\Delta t}\,\sigma(t^k,x)y\Big)\, n^k(x)N(y)dxdy.$$

We cannot obtain a simple equation for n^k from this formula but we can use again Taylor's formula to obtain the approximation

$$\int u(x)n^{k+1}(x)dx = \int\int \Big[u(x) + \Delta t U(t^k,x).Du(x) + \sqrt{\Delta t}\,\sigma\big(t^k,x)y.Du(x) + \tfrac{\Delta t}{2}\sigma(t^k,x)^2y^2\Big]\, n^k(x)N(y)dxdy + O(\Delta t^{3/2}),$$

$$\begin{aligned}\int u(x)n^{k+1}(x)dx &= \int \big[u(x) + \Delta t U(t^k,x).Du(x) + \tfrac{\Delta t}{2}B(t^k,x)\big]\, n^k(x)dx + O(\Delta t^{3/2}) \\ &= \int u(x)\big[n^k(x) - \Delta t \operatorname{div}[U(t^k,x)n^k(x)] \\ &\quad + \tfrac{\Delta t}{2}D^2[B(t^k,x)n^k(x)]\big]\, dx + O(\Delta t^{3/2}).\end{aligned}$$

Because this holds true for all smooth functions u, it means that

$$n^{k+1}(x) = n^k(x) - \Delta t \operatorname{div}[U(t^k,x)n^k(x)] + \frac{\Delta t}{2}D^2[B(t^k,x)n^k(x)] + O(\Delta t^{3/2}).$$

As Δt vanishes, we recover the complete Fokker-Planck equation (8.14). □

When using the Stratonovich integral, that is, the midpoint scheme (8.20), the formalism is similar. This goes as follows (again with $d = p = 1$ to simplify)

$$\begin{aligned}u\big(X^{k+1}\big) &= u\Big(X^k + \Delta t\, U\big(t^k,X^k\big) + \sqrt{\Delta t}\,\sigma\big(t^k, \tfrac{X^k+X^{k+1}}{2}\big)Y^k\Big) \\ &= u\Big(X^k + \Delta t\, U\big(t^k,X^k\big) + \sqrt{\Delta t}\,\sigma\big(t^k,X^k\big)Y^k \\ &\quad + \tfrac{\sqrt{\Delta t}}{2}\sigma'\big(t,X^k\big)(X^{k+1}-X^k)Y^k + O(\Delta^{3/2})\Big) \\ &= u\Big(X^k + \Delta t\, U\big(t^k,X^k\big) + \sqrt{\Delta t}\,\sigma\big(t^k,X^k\big)Y^k \\ &\quad + \tfrac{\Delta t}{2}\sigma'\big(t,X^k\big)\sigma\big(t,X^k\big)(Y^k)^2 + O(\Delta^{3/2})\Big),\end{aligned}$$

(σ' here means the x derivative of $\sigma(t,x)$).

Using again Definition 8.8 for the probability law n^k, this is written

$$\int u(x)n^{k+1}(x)dx = \int\int u\Big(x + \Delta t U(t^k,x) + \sqrt{\Delta t}\,\sigma(t^k,x)y + \frac{\Delta t}{2}\sigma'(t^k,x)\sigma(t^k,x)^2y^2\Big)\, n^k(x)N(y)dxdy + O(\Delta^{3/2}),$$

$$\int u(x)n^{k+1}(x)dx = \int \Big[u(x) + \Delta t U(t^k,x)Du(t^k,x) + \frac{\Delta t}{2}\sigma'(t^k,x)\sigma(t^k,x)Du(t^k,x) + \tfrac{\Delta t}{2}\sigma(t^k,x)^2D^2u(t^k,x)\Big]\, n^k(x)dx + O(\Delta^{3/2}).$$

We pass to the limit as Δt vanishes and find

$$\int u(x)\frac{\partial n(t,x)}{\partial t}dx = \int \Big[U(t,x)Du(t,x) + \frac{1}{2}\sigma'(t,x)\sigma(t,x)Du(t,x) + \frac{1}{2}\sigma(t,x)^2 D^2 u(t,x)\Big]\, n(t,x)dx.$$

We can write after integration by parts and use of the chain rule

$$\int u(x)\tfrac{\partial n(t,x)}{\partial t}dx = \int \Big[\text{div}\big[-[U(t,x) + \tfrac{1}{2}\sigma'(t,x)\sigma(t,x)]n(t,x)\big] + \tfrac{1}{2}D^2[\sigma(t,x)^2 n(t,x)]\Big]\, u(t,x)dx.$$

In other words, the Stratonovich integral, leads to the modified Fokker-Planck equation

$$\frac{\partial n(t,x)}{\partial t} + \text{div}\big[[U(t,x) + \frac{1}{2}\sigma'(t,x)\sigma(t,x)]n(t,x)\big] - \frac{1}{2}D^2[B(t,x).n(t,x)] = 0.$$

8.9 Oriented Collective Motion

As we have seen, the Fokker-Planck Equation is well adapted to describe the motion of a large number of cells (or more generally individuals) that move both with randomness and oriented drift. The drift can result from a signal which itself is emitted by the population; this generates collective behavior of the population.

With these modeling assumptions, we arrive to a nonlinear version of the Fokker-Planck equation

$$\begin{cases} \frac{\partial}{\partial t}n(t,x) - \Delta n(t,x) + \text{div}\big(n(t,x)\nabla S(t,x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ S(t,x) = \int_{\mathbb{R}^d} K(x-y)n(t,y)dy, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.25}$$

The convolution kernel $K(\cdot)$ describes the long range dispersal of the signal emitted by an individual located at y and generating the signal (chemical potential) $S(x)$ at location x. The gradient $\nabla S(x)$ of this potential defines the preferred direction (and intensity) of the active motion of an individual located at x.

Usually, in a homogeneous and isotropic medium, the kernel satisfies $K(x) = \bar{K}(|x|)$. One distinguishes the attractive movement $\bar{K}'(\cdot) \leq 0$ and the case $\bar{K}'(\cdot) \geq 0$ for repulsive movement. In physics when $K(x) = \pm\frac{1}{|x|}$, the former corresponds to Newtonian gravitational forces, the latter to the Coulombic electric force. This can be seen from the exercise below. Figure 8.2 depicts the numerical solution of (8.25)

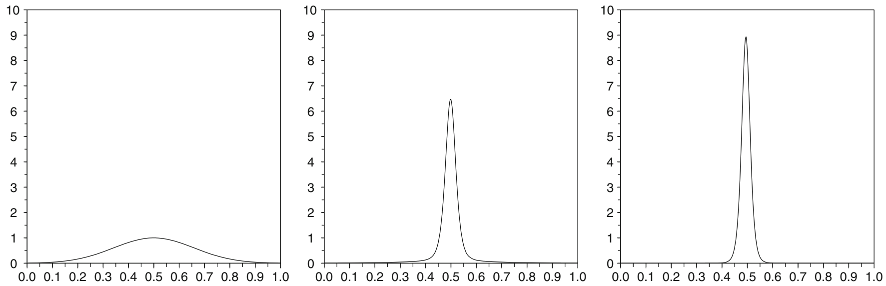

Fig. 8.2 A numerical solution of (8.25) at three different times for an attractive interaction kernel K. Such models have the property to create high concentrations (aggregations)

in the attraction case and $K(x) = \frac{1}{|x|}$. When the total density is sufficiently large the population has a tendency to aggregate and form a spike solution (see Sect. 5.1).

The Keller-Segel system [1, 8, 10, 13] for chemotaxis is the most famous model in this area and assumes that cells move with a combination of a random (Brownian) motion and an oriented drift, which is a chemical gradient of a molecule emitted by the cells themselves and diffused in the medium. Therefore, the Keller-Segel system corresponds to a singular kernel $K(\cdot)$ (the fundamental solution of the Laplace equation). Then, the solution of (8.25) can concentrate in finite time as a Dirac mass as mentioned in Sect. 6.3.

Exercise Assume that $K(x) = \bar{K}(|x|)$.

1. Derive formally the free energy for the solutions of (8.25)

$$\frac{d}{dt}\int_{\mathbb{R}^d} \big[n(t,x)\ln n(t,x) - \frac{1}{2}n(t,x)S(t,x)\big]dx := -D(t) \leq 0$$

   and compute $D(t)$.
2. Compute $E(t)$ for the dynamic of the second moment

$$\frac{d}{dt}\int_{\mathbb{R}^d} \frac{|x|^2}{2} n(t,x)dx = E(t).$$

   Interpret this relation in terms of attractive or repulsive kernels.

Solution

1. $D(t) = \int_{\mathbb{R}^d} n|\nabla(S + \ln n)|^2 dx$.
2. $E(t) = d\int_{\mathbb{R}^d} n^0 + \frac{1}{2}\int_{\mathbb{R}^d\times\mathbb{R}^d} |x-y|\bar{K}'(|x-y|)n(t,x)n(t,y)dx\,dy$.

The contribution $d\int_{\mathbb{R}^d} n^0$ results from the dispersion by Brownian motion. A repulsive potential $K' > 0$ adds up to this effect. On the contrary, an attractive potential $K' < 0$ has tendency to decrease the second moment.

8.10 Nonoriented Collective Motion

Movement can also be completely nonoriented, by this we mean a Brownian motion with variable intensity and thus with a zero mean. Nevertheless, this can generate interesting patterns. This is the case when $U \equiv 0$ in (8.16) but the intensity of the Brownian motion depends on the local population density through a smooth function $\Sigma : \mathbb{R}^+ \to \mathbb{R}$,

$$\sigma(t,x) = \Sigma\big(n(t,x)\big).$$

When the individuals are attracted to (or need) the rest of the population, then $\Sigma'(\cdot) \le 0$, which means that the larger the population, the lower the level of movement. When the individuals do not like high concentrations we take $\Sigma'(\cdot) \ge 0$. The Fokker-Planck equation reduces to the parabolic equation for the density

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \Delta A\big(n(t,x)\big) = 0, \qquad t \ge 0,\ x \in \mathbb{R}^d, \\ A(n) = \frac{1}{2} n \Sigma(n)^2, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.26}$$

In Fig. 8.3, we present the numerical solutions of a relaxation system close to (8.26):

$$\begin{cases} \frac{\partial}{\partial t} n_\varepsilon(t,x) - \frac{1}{2}\Delta[\Sigma^2\big(m_\varepsilon(t,x)\big) n_\varepsilon(t,x)] = 0, \qquad t \ge 0,\ x \in (0,1), \\ -\varepsilon \Delta m_\varepsilon(t,x) + m_\varepsilon(t,x) = n_\varepsilon(t,x), \end{cases} \tag{8.27}$$

together with a Neumann boundary condition for both equations (the total number of individuals remains constant in time). We have computed the case when $\Sigma(\cdot)$ is decreasing near $n = 0$, which means that individuals tend to avoid low densities by moving fast (still with average 0). In our test case

$$A(n) = \frac{n^3}{3} - \frac{n^2}{2} + 2n,$$

and $A'(n) \le$ for $1 \le n \le 2$. This is an unstable region and this creates discontinuities. The constraint for the conservation of total number of individuals, enforces that part of the population has to remain at a low level of density.

This form of equation is also related to models of phase transition and the Stefan problem, see Chap. 10 and Sect. 7.4.

Exercise Define $\Phi(n)$ by $\Phi' = A$. Show that $\int_{\mathbb{R}^d} \Phi\big(n(t,x)\big)dx$ is decreasing. When can it be convex?

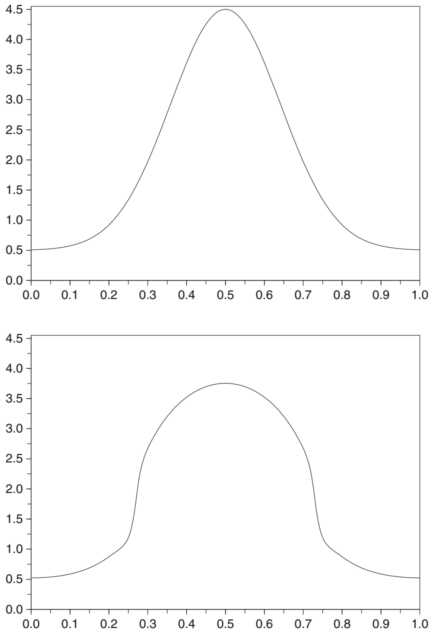

Fig. 8.3 A numerical solution $n(t,x)$ of (8.26), $0 \le x \le 1$ (abscissa), at four different times when $A(n)$ has a decreasing region for $1 \le n \le 2$. *Top left*, the initial data. *Bottom right*, the final time (the steady state is composed of two constant states separated by two discontinuities). In abscissae x, in ordinates $n(t,x)$

Exercise Perform a numerical simulation of the system (8.27) and use a decreasing function Σ. Compare with the results in Fig. 8.3.

8.11 Cross-Diffusion

In ecology, one can encounter aversion between competing species. Each species moves according to pure diffusion (Brownian motion), whose intensity increases with all the densities of all the species present at the same location. This leads to parabolic systems with so-called *cross-diffusions*. One can expect that this effect may lead to segregation of species; species will position spatially so as to avoid each other.

For two interacting species with densities n_1 and n_2, we write that each Brownian motion has an intensity which depends on the densities (n_1, n_2) and this leads to a system of two coupled Fokker-Planck equations

$$\begin{cases} \frac{\partial}{\partial t} n_1(t,x) - \Delta[n_1 \; a_1\big(n_1(t,x), n_2(t,x)\big)] = 0, & t \geq 0, \; x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} n_2(t,x) - \Delta[n_2 \; a_2\big(n_1(t,x), n_2(t,x)\big)] = 0. \end{cases} \tag{8.28}$$

In such models, where the a_i's depend on n_j, second order derivatives of n_j appear in the equation for n_1. This is why they are called cross-diffusions. The subject of cross-diffusions is also very specific and, to gain an insight, some papers are [4, 5, 9, 12].

A strong property is existence of an entropy under the condition for the nonlinearities a_i in (8.28)

$$\left(\frac{\partial a_1}{\partial n_2} + \frac{\partial a_2}{\partial n_1}\right)^2 \leq 4\left[\left(\frac{\partial a_1}{\partial n_1} + \frac{a_1}{n_1}\right)\left(\frac{\partial a_2}{\partial n_2} + \frac{a_2}{n_2}\right)\right], \qquad \frac{\partial a_i}{\partial n_i} \geq 0. \tag{8.29}$$

This is because one can compute

$$\frac{d}{dt}\int_{\mathbb{R}^d} [n_1 \ln n_1 + n_2 \ln n_2] + \int_{\mathbb{R}^d} \left[\frac{|\nabla n_1|^2 a_1}{n_1} + \frac{|\nabla n_2|^2 a_2}{n_2}\right]$$

$$= -\int_{\mathbb{R}^d} \Bigg[|\nabla n_1|^2 \frac{\partial a_1}{\partial n_1} + \left(\frac{\partial a_1}{\partial n_2} + \frac{\partial a_2}{\partial n_1}\right) \nabla n_1.\nabla n_2 + |\nabla n_2|^2 \frac{\partial a_2}{\partial n_2}\Bigg]$$

and the right hand side is negative under the condition (8.29).

A famous competition system (that includes reaction terms) was proposed by Shigesada et al. [14]

$$\begin{cases} \frac{\partial}{\partial t} n_1 - \Delta[(d_1 + \alpha_1 n_1 + \beta_1 n_2) n_1] = (r_1 - c_{11} n_1 - c_{12} n_2) n_1, \\ \frac{\partial}{\partial t} n_2 - \Delta[(d_2 + \beta_2 n_1 + \alpha_2 n_2) n_2] = (r_2 - c_{21} n_1 - c_{22} n_2) n_2. \end{cases}$$

L. Chen and A. Jüngel [3] have developed a theory for this system under a more general condition than (8.29). They introduced a variant of the above entropy inequality, namely, discarding the left hand side (in other words, $r_i = 0$, $c_{ij} = 0$), we have

$$\frac{d}{dt}\int_{\mathbb{R}^d} \left[\frac{n_1}{\beta_1} \ln n_1 + \frac{n_2}{\beta_2} \ln n_2\right] \leq 0,$$

which holds under the simple sign condition $d_i \geq 0$, $\alpha_i \geq 0$, $\beta_i > 0$.

References

1. Baker, R.E., Gaffney, E.A., Maini, P.K.: Partial differential equations for self-organization in cellular and developmental biology. Nonlinearity **21**, R251–R290 (2008)
2. Brezis, H.: Analyse Fonctionnelle, Théorie et Applications. Masson, Paris (1983)
3. Chen, L., Jüngel, A.: Analysis of a parabolic cross-diffusion population model without self-diffusion. J. Differ. Equ. **224**(1), 39–59 (2006)
4. Desvillettes, L., Fellner, K., Pierre, M., Vovelle, J.: Global existence for quadratic systems of reaction-diffusion. Adv. Nonlinear Stud. **7**(3), 491–511 (2007)
5. Desvillettes, L., Lepoutre, T., Moussa, A.: Entropy, duality and cross-diffusion. SIAM J. Math. Anal. **46**(1), 820–853 (2014)
6. Evans, L.C.: Partial Differential Equations. Graduate Studies in Mathematics, vol. 19. American Mathematical Society, Providence (1998)
7. Gilbarg, D., Trudinger, N.: Elliptic Partial Differential Equations of Second Order, 2nd edn. Springer, Berlin (2003)
8. Hillen, T., Painter, K.: A user's guide to PDE models for chemotaxis. J. Math. Biol. **58**(1), 183–217 (2009)
9. Iida, M., Mimura, M., Ninomiya, H.: Diffusion, cross-diffusion and competitive interaction. J. Math. Biol. **53**(3), 617–641 (2006)
10. Keller, E.F., Segel, L.A.: Model for chemotaxis. J. Theor. Biol. **30**, 225–234 (1971)
11. Ledoux, M.: The Concentration of Measure Phenomenon. AMS Mathematical Surveys and Monographs, vol. 89. American Mathematical Society, Providence (2001)
12. Lou, Y., Martinez, S.: Evolution of cross-diffusion and self-diffusion. J. Biol. Dyn. **3**(4), 410–429 (2009)
13. Perthame, B.: Transport equations arising in biology. L. N. series 'Frontiers in Mathematics'. Birkhauser, Basel (2007)
14. Shigesada, N., Kawasaki, K., Teramoto, E.: Spatial segregation of interacting species. J. Theor. Biol. **79**(1), 83–99 (1979)

Chapter 9
From Jumps and Scattering to the Fokker-Planck Equation

Scattering equations are integral equations closely related to the Fokker-Planck equations, as we shall see, but simpler to analyze. They come from physics (neutron transport equations, wave scattering) but also from adaptive evolution, representing mutations of organisms during reproduction, or in bacterial runs and tumbling movements (the microscopic description of chemotaxis, [2, 3]). More generally, in relation to probability, they are the Kolmogorov equations for the probability density of jump processes.

9.1 The Scattering Equation

9.1.1 The Integral Model

We depart from the simple ordinary differential equation (in infinite dimension)

$$\frac{\partial}{\partial t} n(t,x) + k(x)n(t,x) = \int_{\mathbb{R}^d} K(y, x-y)n(t,y)dy, \qquad t \geq 0,\ x \in \mathbb{R}^d, \tag{9.1}$$

together with an initial data $n^0 \in L^1(\mathbb{R}^d)$. We use the assumption and notation,

$$K(y,z) \geq 0, \qquad k(y) := \int_{\mathbb{R}^d} K(y,z)dz \in L^\infty(\mathbb{R}^d). \tag{9.2}$$

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_9

This scattering equation shares properties with the Fokker-Planck equation, namely we have

$$n^0 \geq 0 \implies n \geq 0, \tag{9.3}$$

$$\int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} n^0(x)dx, \quad \forall t \geq 0, \tag{9.4}$$

$$\int_{\mathbb{R}^d} |n(t,x)|dx \leq \int_{\mathbb{R}^d} |n^0(x)|dx, \quad \forall t \geq 0. \tag{9.5}$$

However, there is not always a simple formula for the steady state (see Sect. 9.2 for explicit constructions).

9.1.2 Existence of Solutions of the Scattering Equation

The existence and uniqueness of solutions of (9.1) is a simple consequence of the Cauchy-Lipschitz theorem.

Lemma 9.1 *Assume* (9.2)*, then for* $n^0 \in L^1(\mathbb{R}^d)$*, there is a unique solution* $n \in C\big(\mathbb{R}^+; L^1(\mathbb{R}^d)\big)$ *of* (9.1) *and the properties* (9.3)–(9.5) *hold true.*

Proof We first prove that the linear operator $n \mapsto k(x)n(x) - \int_{\mathbb{R}^d} K(y, x-y)n(y)dy$ is Lipschitz continuous from L^1 into L^1. That is because

$$\|k(\cdot)n(\cdot)\|_{L^1(\mathbb{R}^d)} \leq \|k\|_{L^\infty(\mathbb{R}^d)} \; \|n\|_{L^1(\mathbb{R}^d)},$$

$$\begin{aligned} &\| \int_{\mathbb{R}^d} K(y, \cdot - y)n(y)dy\|_{L^1(\mathbb{R}^d)} \\ &\quad \leq \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(y, x-y)|n(y)|dy\, dx \leq \|k\|_{L^\infty(\mathbb{R}^d)} \; \|n\|_{L^1(\mathbb{R}^d)}. \end{aligned}$$

Then, we may apply the Cauchy-Lipschitz theorem; in the Banach space $L^1(\mathbb{R}^d)$ a Lipschitz continuous differential equation has a unique global classical solution $n \in C^1\big(\mathbb{R}^+; L^1(\mathbb{R}^d)\big)$.

The Lebesgue theorem for derivatives also shows that

$$\frac{d}{dt}\int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} \left[\int_{\mathbb{R}^d} K(y, x-y)n(t,y)dy - k(x)n(t,x) \right] dx = 0,$$

which gives mass conservation identity (9.4).

To include the sign and prove (9.5), we use the method of Stampacchia, see Sect. 3.3. We introduce a family $H_\delta(\cdot)$ of smooth, non-decreasing and convex functions such that $H'_\delta(\cdot) \le 1$ and $H_\delta(\cdot) \nearrow H(\cdot) = \mathrm{sgn}_+(\cdot)$. We have

$$\tfrac{\partial}{\partial t} H_\delta(n(t,x)) + k(x)H'_\delta(n(t,x))n(t,x) = H'_\delta(n(t,x)) \textstyle\int_{\mathbb{R}^d} K(y, x-y)n(t,y)dy$$
$$\le \textstyle\int_{\mathbb{R}^d} K(y, x-y)n_+(t,y)dy.$$

Therefore, in the limit $\delta \to 0$,

$$\frac{\partial}{\partial t} n_+(t,x)dx + k(x)n_+(t,x) \le \int_{\mathbb{R}^d} K(y, x-y)n_+(t,y)dy,$$

and

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_+(t,x)dx \le 0.$$

Therefore, when n^0 is nonpositive, it remains nonpositive and, applying to $-n^0$ we find (9.3).

The L^1 contraction (9.5) follows with the combination $-n + 2n_+ = |n|$. □

9.2 The Relative Entropy

As all linear problems that satisfy a positivity principle, the scattering equation has a family of relative entropies. We assume that there exists a positive steady state

$$\exists N(x) > 0, \text{ such that } k(x)N(x) = \int_{\mathbb{R}^d} K(y, x-y)N(y)dy. \tag{9.6}$$

Semi-explicit examples, where one can prove the existence of such steady states, are given as an exercise at the end of this paragraph. An explicit example is the projection operator; being given $N(x) > 0$ with $\int_{\mathbb{R}^d} N = 1$, we choose a weight $\bar{k}$ such that $\int \bar{k}(y)N(y)dy = 1$ and take K as

$$K(y, x-y) = \bar{k}(y)k(x)N(x).$$

There is another and larger class of examples of kernels K where N is known. Still being given $N(x) > 0$ with $\int_{\mathbb{R}^d} N = 1$ and a symmetric kernel $\tilde{K}(x,y) = \tilde{K}(y,x) > 0$, we take K as

$$K(y, x-y) = \frac{\tilde{K}(x,y)}{N(y)}, \qquad k(y) := \int \frac{\tilde{K}(x,y)}{N(y)}dx$$
$$\Longleftrightarrow k(x)N(x) = \int \tilde{K}(y,x)dy = \int \tilde{K}(x,y)dy.$$

Theorem 9.2 (Relative Entropy for the Scattering Equation) *For all convex function $H(\cdot)$, one has*

$$\frac{d}{dt}\int_{\mathbb{R}^d} N(x)H\left(\frac{n(t,x)}{N(x)}\right) := -D_H^{sc}(n|N) \le 0,$$

$$D_H^{sc}(n|N) = \int_{\mathbb{R}^d\times\mathbb{R}^d} K(y,x-y)N(y)\left[H\left(\frac{n(t,y)}{N(y)}\right) - H\left(\frac{n(t,x)}{N(x)}\right)\right.$$
$$\left. -H'\left(\frac{n(t,x)}{N(x)}\right)\left(\frac{n(t,y)}{N(y)} - \frac{n(t,x)}{N(x)}\right)\right] dx\, dy.$$

Proof Left to the reader (see [2]). □

Corollary 9.3 *Assume that $n^0 \le C^0 N$, then for all $t \ge 0$,*

$$n(t,x) \le C^0 N.$$

Exercise The aim of this exercise is to find a class of kernels for which a positive steady state $N(x)$ exists in (9.6). We give, for $i = 1,\ 2, \dots, I$ functions

$$P_i > 0, \qquad Q_i > 0, \qquad \int_{\mathbb{R}^d} P_i(x)dx = 1, \qquad Q_i \in L^\infty(\mathbb{R}^d).$$

We define

$$k(x) = \sum_{i=1}^{I} Q_i(x), \qquad K(y,x-y) = \sum_{i=1}^{I} P_i(x)Q_i(y).$$

We aim to find $\alpha_i > 0$ such that $N(x) = \sum_{i=1}^{I} \alpha_i \frac{P_i(x)}{k(x)}$ is the steady state.

1. Show that $N(x)$ is a steady state if, and only if, $\sum_{j=1}^{I} A_{ij}\alpha_j = \alpha_i$, $\forall i = 1,..,I$ with the matrix having positive entries

$$A_{ij} = \int_{\mathbb{R}^d} \frac{P_j(y)}{k(y)} Q_i(y)dy > 0.$$

2. Using the Perron-Froebenius theorem, show that there is a unique $\lambda > 0$ and $\alpha_i > 0$, $i = 1, .., I$ such that

$$\sum_{j=1}^{I} A_{ij}\alpha_j = \lambda\alpha_i.$$

3. Prove that $\lambda = 1$ and conclude.

Hint. $\sum_{i=1}^{I} A_{ij} = 1$.

9.3 The Hyperbolic Limit of Scattering

We can derive the transport equation (8.11) from the scattering equation and we begin with this because it is simpler than the derivation of the complete Fokker-Planck equation.

Hyperbolic Rescaling To achieve this goal, we assume that scattering occurs with small changes and a fast rate (in other words, we change the time scale according to the size of the jumps)

$$\begin{cases} \frac{\partial}{\partial t} n_\varepsilon(t,x) + \frac{1}{\varepsilon}\left[k(x)n_\varepsilon(t,x) - \int_{\mathbb{R}^d} \frac{1}{\varepsilon^d} K(y, \frac{x-y}{\varepsilon}) n_\varepsilon(t,y)dy\right] = 0, \\ n_\varepsilon(t=0,x) = n^0(x), \qquad \int_{\mathbb{R}^d} |n^0(x)|dx =: M^0. \end{cases} \tag{9.7}$$

Additionally to (9.2), we define and assume

$$U(x) := \int_{\mathbb{R}^d} zK(x,z)dz \in L^\infty(\mathbb{R}^d), \qquad \sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |z|^2 K(x,z)dz < \infty. \tag{9.8}$$

Based only on the bound $\int_{\mathbb{R}^d} |n_\varepsilon(t,x)|dx = M^0$ for all $t \geq 0$, we can extract from n_ε a subsequence such that for all $T > 0$,

$$n_\varepsilon \rightharpoonup n \qquad \text{weakly in measures in } \ [0,T] \times \mathbb{R}^d.$$

it means that for $\Phi \in C_c\big(\mathbb{R}^+ \times \mathbb{R}^d\big)$,

$$\int_0^\infty \int_{\mathbb{R}^d} n_\varepsilon(t,x)\Phi(t,x)dx\, dt \underset{\varepsilon\to 0}{\longrightarrow} \int_0^\infty \int_{\mathbb{R}^d} n(t,x)\Phi(t,x)dx\, dt.$$

With this material at hand, we can handle measure solutions to the limiting problem compatible only with a continuous velocity field U and uniform limits in the integrals involved in (9.8).

We can prefer stronger estimates based on relative entropy, see Sect. 9.2. Then, we assume that for a function $\overline{N} \in L^1 \cap L^\infty(\mathbb{R}^d)$, the initial data and the steady states N_ε in (9.6) undergo uniform control

$$|n^0| \leq C_0 N_\varepsilon \leq \overline{N}.$$

This implies the same control at later times

$$|n(t,\cdot)| \leq C_0 N_\varepsilon \leq \overline{N}.$$

Then we may extract a subsequence such that

$$n_\varepsilon \rightharpoonup n \quad \text{in } L^\infty(\mathbb{R}^+ \times \mathbb{R}^d) - w*, \quad |n| \leq \overline{N}. \tag{9.9}$$

This means that for $\Phi \in L^1\big(\mathbb{R}^+ \times \mathbb{R}^d\big)$,

$$\int_0^T \int_{\mathbb{R}^d} n_\varepsilon(t,x)\Phi(t,x)dx\,dt \underset{\varepsilon\to 0}{\longrightarrow} \int_0^T \int_{\mathbb{R}^d} n(t,x)\Phi(t,x)dx\,dt.$$

This assumption for n^0 and N_ε is rather restrictive although an example is built in Sect. 9.5.

In Sect. 9.6 we show that we can go further. With some simple regularity assumptions for K, we derive more general L^2 bounds. We take them for granted here.

The Hyperbolic Limit With this in mind, we can extract from n_ε a subsequence that converges weakly in $L^2\big((0,T) \times \mathbb{R}^d\big)$ for all $T > 0$, to n

$$n \in L^\infty\big(\mathbb{R}^+; L^1 \cap L^2(\mathbb{R}^d)\big).$$

Theorem 9.4 (Hyperbolic Limit for the Scattering Equation) *Assume* (9.2), (9.8) *and for all* $T > 0$, $\sup_{0\leq t\leq T} \|n(t)_\varepsilon\|_{L^2(\mathbb{R}^d)} \leq C(T)$. *After extraction, the weak* L^2*-limit* n *of the solution of* (9.7) *satisfies, in the distributional sense, the transport equation*

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) + \operatorname{div}\big(n(t,x)U(t,x)\big) = 0, & t \geq 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{9.10}$$

Proof We change variables from y to $z = \frac{x-y}{\varepsilon}$ and arrive to the formulation

$$\frac{\partial}{\partial t} n_\varepsilon(t,x) + \frac{1}{\varepsilon} k(x) n_\varepsilon(t,x) = \frac{1}{\varepsilon} \int K(x - \varepsilon z, z) n_\varepsilon(t, x - \varepsilon z)dz.$$

Using the property (9.2), this is also written

$$\frac{\partial}{\partial t} n_\varepsilon(t,x) = -\int \frac{1}{\varepsilon}\big[K(x,z) n_\varepsilon(t,x) - K(x-\varepsilon z, z) n_\varepsilon(t, x-\varepsilon z)\big] dz.$$

We introduce a test function $\Phi(t,x) \in C^2(\mathbb{R}^+ \times \mathbb{R}^d)$ with compact support that is $\Phi(t,x) = 0$ for $t \geq T$ or $|x| > R$ for some $T,\ R > 0$. We multiply this equation by $\Phi(t,x)$ and integrate in $t,\ x$. We find, after using the Fubini theorem,

$$\begin{aligned}
&-\int_0^T \int_{\mathbb{R}^d} \frac{\partial}{\partial t}\Phi(t,x) n_\varepsilon(t,x) - \int_{\mathbb{R}^d} \Phi(0,x) n^0(x) dx \\
&= -\int_0^T \int_{\mathbb{R}^d} n_\varepsilon(t,x) \int_{\mathbb{R}^d} K(x,z) \frac{\Phi(t,x) - \Phi(t,x+\varepsilon z)}{\varepsilon} dz\, dx \\
&= -\int_0^T \int_{\mathbb{R}^d} n_\varepsilon(t,x) \int_{|z|<R} K(x,z) \frac{\Phi(t,x) - \Phi(t,x+\varepsilon z)}{\varepsilon} dz\, dx + I_\varepsilon^R.
\end{aligned}$$

It remains to handle these two terms. On the one hand

$$I_\varepsilon^R = -\int_0^T \int_{\mathbb{R}^d} n_\varepsilon(t,x) \int_{|z|\geq R} K(x,z) \frac{\Phi(t,x) - \Phi(t,x+\varepsilon z)}{\varepsilon} dz\, dx,$$

and we can control it using the second moment in (9.8)

$$\begin{aligned}
|I_\varepsilon^R| &\leq \int_0^T \int_{\mathbb{R}^d} |n_\varepsilon(t,x)| dx \ \sup_{x\in\mathbb{R}^d} \int_{|z|\geq R} K(x,z) \frac{|\Phi(t,x) - \Phi(t,x+\varepsilon z)|}{\varepsilon} dz dt \\
&\leq T\, M^0 \|\nabla\Phi\|_{L^\infty(\mathbb{R}^d)} \ \sup_{x\in\mathbb{R}^d} \int_{|z|\geq R} K(x,z)|z| dz \\
&\leq \tfrac{T\, M^0}{R} \ \|\nabla\Phi\|_{L^\infty(\mathbb{R}^d)} \ \sup_{x\in\mathbb{R}^d} \int_{|z|\geq R} K(x,z)|z|^2 dz \\
&\leq \tfrac{C}{R}
\end{aligned}$$

for a constant C independent of ε.

On the other hand, strongly in $L^2\big((0,T)\times\mathbb{R}^d\big)$, we have the limit

$$\int_{|z|<R} K(x,z) \frac{\Phi(t,x) - \Phi(t,x+\varepsilon z)}{\varepsilon} dz \underset{\varepsilon\to 0}{\longrightarrow} -\int_{|z|<R} K(x,z) z.\nabla\Phi(t,x) dz$$

and thus by weak-strong convergence we find

$$\begin{aligned}
&-\int_0^T \int_{\mathbb{R}^d} \frac{\partial}{\partial t}\Phi(t,x) n(t,x) - \int_{\mathbb{R}^d} \Phi(0,x) n^0(x) dx \\
&\qquad\qquad = \int_0^T \int_{\mathbb{R}^d} n(t,x) \int_{|z|<R} K(x,z) z.\nabla\Phi(t,x) dz\, dx + 0\big(\frac{1}{R}\big).
\end{aligned}$$

It remains to pass to the limit as $R \to \infty$ and we find

$$\int_{|z|<R} K(x,z)z.\nabla\Phi(t,x)dz \underset{R\to\infty}{\longrightarrow} U(x).\nabla\Phi(t,x).$$

We finally conclude that

$$-\int_0^T \int_{\mathbb{R}^d} \frac{\partial}{\partial t}\Phi(t,x)n(t,x) - \int_{\mathbb{R}^d} \Phi(0,x)n^0(x)dx = \int_0^T \int_{\mathbb{R}^d} n(t,x)U(x).\nabla\Phi(t,x)dx.$$

This is the weak formulation of Eq. (9.10). □

9.4 The Diffusive Limit of Scattering

The same ideas are involved in the derivation of the complete Fokker-Planck equation (8.14) (including a diffusion matrix) from the scattering equations with a two scale limit.

9.4.1 Rescaling

To do so, we introduce a stronger and balanced scale as follows

$$\frac{\partial}{\partial t}n_\varepsilon(t,x) + \frac{1}{\varepsilon^2}\left[k(x)n_\varepsilon(t,x) - \int_{\mathbb{R}^d} \frac{1}{\varepsilon^d}K_\varepsilon(y, \frac{x-y}{\varepsilon})n_\varepsilon(t,y)dy\right] = 0 \tag{9.11}$$

still with an initial data $n^0 \in L^1(\mathbb{R}^d)$. The kernel K_ε depends only slightly on ε; we have in mind here a small asymmetry. Specifically, we make the assumptions,

$$K_\varepsilon(y,z) \geq 0, \qquad k(y) := \int_{\mathbb{R}^d} K_\varepsilon(y,z)dz \in L^\infty(\mathbb{R}^d), \tag{9.12}$$

$$\int_{\mathbb{R}^d} (1+|z|^3)K_\varepsilon(y,z)dz \in L^\infty(\mathbb{R}^d), \tag{9.13}$$

$$\int_{\mathbb{R}^d} zK_\varepsilon(y,z)dz = \varepsilon U(y), \qquad \int_{\mathbb{R}^d} z_i z_j K_\varepsilon(y,z)dz = B_{ij}(y), \tag{9.14}$$

$$U_i,\ B_{ij} \in C \cap L^\infty(\mathbb{R}^d), \qquad (B_{ij}) \text{ is a definite positive matrix}, \tag{9.15}$$

(here $i,\ j = 1,\dots,I$). Notice that $A_{ij}(x)$ is a symmetric matrix by virtue of its construction.

We again take for granted the L^2 estimates from Sect. 9.6.

Theorem 9.5 *After extraction, the L^2-weak limit n of the solution n_ε of (9.11) satisfies, in the distributional sense, the complete Fokker-Planck equation*

$$\frac{\partial}{\partial t}n(t,x) - \frac{1}{2}\sum_{i,j=1}^{I}\frac{\partial^2}{\partial_{x_i}\partial_{x_j}}\big[B_{ij}(x)n(t,x)\big] + \operatorname{div}\big[U(x)n(t,x)\big] = 0, \tag{9.16}$$

with the initial data n^0.

Proof We proceed as in Sect. 9.3 for the hyperbolic limit and change the variables from y to $z = \frac{x-y}{\varepsilon}$. We arrive to the formulation

$$\frac{\partial}{\partial t}n_\varepsilon(t,x) + \int \frac{1}{\varepsilon^2}\big[K_\varepsilon(x,z)n_\varepsilon(t,x) - K_\varepsilon(x-\varepsilon z,z)n_\varepsilon(t,x-\varepsilon z)\big]dz = 0.$$

We introduce a test function $\Phi(t,x) \in C^3(\mathbb{R}^+ \times \mathbb{R}^d)$ with compact support that is $\Phi(t,x) = 0$ for $t \geq T$ or $|x| > R$ for some $T,\ R > 0$. We find

$$-\int \frac{\partial}{\partial t}\Phi(t,x)n_\varepsilon(t,x) + \int n_\varepsilon(t,x)\int K_\varepsilon(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon^2}dz\,dx$$
$$= \int \Phi(0,x)n^0(x)dx.$$

By a third order Taylor expansion, and thanks to our third moment bounds in assumption (9.13), we can write

$$\int\int_{|z]<R} n_\varepsilon(t,x)K_\varepsilon(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon^2}dz\,dx$$
$$= \int\int_{|z]<R} n_\varepsilon(t,x)K_\varepsilon(x,z)\left[-\frac{z.\nabla\Phi(t,x)}{\varepsilon} - \frac{z_iz_j}{2}D^2_{ij}\Phi(t,x)\right]dz\,dx + O(\varepsilon).$$

We may pass to the limit (here we have to use more, namely that $U^R = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\int_{|z]<R} zK_\varepsilon(x,z)dz$ exists strongly in L^2) and we find

$$\int\int_{|z]<R} n_\varepsilon(t,x)K_\varepsilon(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon^2}dz\,dx$$
$$\underset{\varepsilon\to 0}{\longrightarrow}\int\int_{|z]<R} n(t,x)\left[-U^R.\nabla\Phi(t,x) - \frac{B^R_{i,j}}{2}D^2_{ij}\Phi(t,x)\right]dz\,dx$$

with $B^R_{i,j} = \lim_{\varepsilon\to 0}\int_{|z]<R} K_\varepsilon(x,z)z_iz_jdz.$

The tail, corresponding to large values of $|z|$, has also to be controlled, a difficulty we avoid by assuming that $K(y,z)$ has a bounded support in z.

With this, the exponent R is not present, and we arrive at

$$-\int \frac{\partial}{\partial t}\Phi(t,x)n(t,x) + \int n(t,x)\left[-U(x).\nabla\Phi(t,x)\big((0,T)\times\mathbb{R}^d)\big)\right]$$
$$\left[-\frac{1}{2}B_{ij}(x)D^2_{ij}\Phi(t,x)\right]dx = \int \Phi(0,x)n^0(x)dx.$$

This is the weak formulation of the complete Fokker-Planck equation (9.16). □

9.5 Construction of the Kernel in Scattering Equation

One can also address the reverse question: being given the coefficients $U(\cdot) \in L^\infty(\mathbb{R}^d)^d$ and $B(\cdot) \in L^\infty(\mathbb{R}^d)^{d\times d}$, a definite positive symmetric matrix, is it possible to build a suitable kernel K_ε that gives the moments in (9.13), (9.14)? To do so, it is sufficient to choose $k(y) \equiv 1$ and to use the formula

$$K_\varepsilon(y,z) = \det B^{-1/2}\,\mathcal{K}\left(\left|B(y)^{-1/2}.(z-\varepsilon U(y))\right|^2\right),$$

where we choose for $B(y)^{-1/2}$ the unique definite, positive symmetric matrix, such that $B(y)^{-1/2}.B(y)^{-1/2} = B(y)^{-1}$. And for $\mathcal{K}:\mathbb{R}^+ \to \mathbb{R}^+$we choose a smooth function such that

$$\int_{\mathbb{R}^d}\mathcal{K}(|z|^2)dz = 1, \qquad \int_{\mathbb{R}^d} z\mathcal{K}(|z|^2)dz = 0, \qquad \int_{\mathbb{R}^d} z_i z_j\mathcal{K}(|z|^2)dz = \delta_{ij},$$

for example a normalized Gaussian will do it.

Indeed, after the change of variable $z \mapsto \eta = B(y)^{-1/2}.(z-\varepsilon U(y))$, $d\eta = \det B^{-1/2}(y)\; dz$, one can compute successively

$$\int_{\mathbb{R}^d} K_\varepsilon(y,z)dz = \int_{\mathbb{R}^d}\mathcal{K}(|\eta|^2)d\eta = 1,$$

$$\int_{\mathbb{R}^d} zK_\varepsilon(y,z)dz = \varepsilon U(y)\int_{\mathbb{R}^d}K_\varepsilon(y,z)dz + \int_{\mathbb{R}^d}(z-\varepsilon U(y))K_\varepsilon(y,z)dz = \varepsilon U(y),$$

because,

$$\int_{\mathbb{R}^d}(z-\varepsilon U(y))K_\varepsilon(y,z)dz = \int_{\mathbb{R}^d} B(y)^{1/2}.\eta\mathcal{K}\left(|\eta|^2\right)d\eta = 0.$$

Finally, we also compute using the previous relations

$$\int_{\mathbb{R}^d} z_i z_j K_\varepsilon(y,z)dz = \int_{\mathbb{R}^d}(z_i - \varepsilon U_i(y))(z_j - \varepsilon U_j(y))K_\varepsilon(y,z)dz - \varepsilon^2 U_i(y)U_j(y)$$
$$= \int_{\mathbb{R}^d} (B(y)^{1/2}.\eta)_i.(B(y)^{1/2}.\eta)_j\, \mathcal{K}\left(|\eta|^2\right) d\eta - \varepsilon^2 U_i(y)U_j(y)$$
$$= B_{ij}(y) - \varepsilon^2 U_i(y)U_j(y)$$

because

$$\int_{\mathbb{R}^d} (B(y)^{1/2}.\eta)_i.(B(y)^{1/2}.\eta)_j\, \mathcal{K}\left(|\eta|^2\right) d\eta = \sum_{k,l} \int_{\mathbb{R}^d} (B(y)^{1/2}_{ik}.\eta_k\, B(y)^{1/2}_{lj}.\eta_l\, \mathcal{K}\left(|\eta|^2\right) d\eta$$
$$= \sum_k (B(y)^{1/2}_{ik}\, B(y)^{1/2}_{kj} = B_{ij}(y).$$

This is not exactly the second relation (9.14) because of the term $-\varepsilon^2 U_i(y)U_j(y)$. However, this is not a real difficulty, we can either change B_{ij} in our construction and replace it by $B_{ij} + \varepsilon^2 U_i(y)U_j(y)$, or notice that a correction in ε^2 does not change the limit in Theorem 9.5.

9.6 Further A Priori Estimates of n_ε

At the expense of more restrictive assumptions we may derive directly, stronger bounds than L^1 for solution of the scattering equation and find that the weak limit in the sections above are indeed in L^2-weak. This uses assumptions that differ in the hyperbolic and parabolic scales.

9.6.1 The Hyperbolic Scale

To do so, and having in mind the hyperbolic scale in (9.7), we assume

$$\int_{\mathbb{R}^d} \big[K(y+\varepsilon z, z) - K(y,z)\big]dz \le \varepsilon L_1. \tag{9.17}$$

Lemma 9.6 *Assume* (9.2), (9.17) *then for all times* $t \ge 0$, *the solution of* (9.7) *satisfies*

$$\|n_\varepsilon(t)\|_{L^2(\mathbb{R}^d)} \le \|n^0\|_{L^2(\mathbb{R}^d)} e^{L_1 t}.$$

Proof We compute from (9.7), and using the change of variable $y \mapsto z = \frac{x-y}{\varepsilon}$,

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx + \frac{1}{\varepsilon}\int_{\mathbb{R}^d} k(x) n_\varepsilon(t,x)^2 dx \\
&= \frac{1}{\varepsilon^{d+1}}\int_{\mathbb{R}^d} K(y, \frac{x-y}{\varepsilon}) n_\varepsilon(t,y) n_\varepsilon(t,x) dy dx \\
&= \int_{\mathbb{R}^d} K(x-\varepsilon z, z) n_\varepsilon(t, x-\varepsilon z) n_\varepsilon(t,x) dz dx \\
&\le \frac{1}{2}\int_{\mathbb{R}^d} K(x-\varepsilon z, z)\big[n_\varepsilon(t, x-\varepsilon z)^2 + n_\varepsilon(t,x)^2\big] dz dx.
\end{aligned}$$

Because $\int_{\mathbb{R}^d} K(x-\varepsilon z, z) n_\varepsilon(t, x-\varepsilon z)^2 dx = \int_{\mathbb{R}^d} K(x,z) n_\varepsilon(t,x)^2 dx$, using (9.2), this reduces to

$$\begin{aligned}
\tfrac{d}{dt}\textstyle\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx &\le \int_{\mathbb{R}^d} \frac{K(x-\varepsilon z, z) - K(x,z)}{\varepsilon} n_\varepsilon(t,x)^2 dz dx \\
&\le L_1 \int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx.
\end{aligned}$$

The Gronwall lemma gives the conclusion. □

9.6.2 The Diffusive Scale

We turn now to assumptions compatible with the diffusive limit and the scaling in (9.11). We consider a second order expansion of K_ε together with (9.14) and assume

$$\left(\int_{\mathbb{R}^d} K_\varepsilon(x-\varepsilon z, z) dz - k(x)\right)_+ \le L_2 \varepsilon^2. \tag{9.18}$$

To understand what this means, we may perform Taylor's expansion and write

$$\begin{aligned}
\tfrac{1}{\varepsilon^2}\big[\textstyle\int_{\mathbb{R}^d} K_\varepsilon(x-\varepsilon z, z) dz - k(x)\big] &= \textstyle\int_{\mathbb{R}^d} \frac{K_\varepsilon(x-\varepsilon z, z) dz - K(x,z)}{\varepsilon^2} dz \\
&\approx \textstyle\int_{\mathbb{R}^d} \big[-\frac{\nabla_x K_\varepsilon(x,z) z}{\varepsilon} + \frac{1}{2} z \otimes z D_x^2 K_\varepsilon(x,z)\big] dz,
\end{aligned}$$

which implies, using the notation (9.14), that

$$\left(-\mathrm{divU} + \frac{1}{2}\sum_{i,j} D_{ij}^2 B_{ij}\right)_+ \in L^\infty(\mathbb{R}^d). \tag{9.19}$$

Exercise Derive L^2 estimates in x for the complete Fokker-Planck equation (9.16) using the assumption (9.19) as in Sect. 8.1.

Proposition 9.7 *With the assumption* (9.2)*,* (9.18)*, we have*

$$\|n_\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \leq \|n^0(\cdot)\|_{L^2(\mathbb{R}^d)} e^{L_2 t}.$$

Proof We compute as before

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx$$
$$= \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^{2d}} K(x-\varepsilon z, z) n_\varepsilon(t, x-\varepsilon z) n_\varepsilon(t,x) dz\, dx - \int_{\mathbb{R}^d} k(x) n_\varepsilon(t,x)^2 dx\right].$$

Since $n_\varepsilon(t,x-\varepsilon z)n_\varepsilon(t,x) \leq \frac{1}{2}[n_\varepsilon(t,x-\varepsilon z)^2 + n_\varepsilon(t,x)^2]$, we have, using (9.12),

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^{2d}} K(x-\varepsilon z, z) n_\varepsilon(t,x)^2 dz\, dx - \int_{\mathbb{R}^d} k(x) n_\varepsilon(t,x)^2 dx\right].$$

Now, using (9.18), we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx \leq L_2 \int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx,$$

and the result follows again from the Gronwall lemma. □

9.7 The Chemical Master Equation

Chemical reactions are derived through an asymptotic analysis similar to that derived above. We explain roughly the formalism using the notations in D. Gillespie [1].

For N molecular species labeled as $i = 1,..,N$ (therefore $d = N$ to fit our notations), $X_i(t) \in \mathbb{N}$ is the number of molecules of species i at time t, and $X(t) = \big(X_1(t),\dots,X_N(t)\big)$ is the molecular population vector.

The index $j = 1,\dots,M$ represents reaction channels. For the reaction indexed by j, $a_j(x) \geq 0$ is the reaction rate (sometimes called propensity function). It is associated with the state-change vector $\nu_j = \big(\nu_{j1},\dots,\nu_{j,N}\big)$, $j = 1,\dots,M$, where $\nu_{ji} \in \mathbb{Z}$ is the change in number of molecular species i produced by reaction j.

The probability to find the system in state $X(t) = x \in \mathbb{N}^N$ at time t is $p(t, x)$. The generator of the jump Markov process for the molecules gives the *chemical master equation*

$$\frac{\partial}{\partial t} p(t,x) = \sum_{j=1}^{M} \big[a_j(x-\nu_j)p(t,x-\nu_j) - a_j(x)p(t,x)\big], \qquad x \in \mathbb{N}^N,\ t \geq 0. \tag{9.20}$$

For a large number of molecules in each species, and ν_j of the order of 1 (that is $X_i \gg \nu_j$), we may rescale according to the small parameter $\varepsilon = \nu/X$. Then, we consider that x is a continuous variable and $\nu = 0(\varepsilon)$. We arrive at the formalism

$$\frac{\partial}{\partial t} p(t,x) = \sum_{j=1}^{M} \big[a_j(x-\varepsilon\nu_j)p(t,x-\varepsilon\nu_j) - a_j(x)p(t,x)\big], \qquad x \in \mathbb{R}^N,\ t \geq 0.$$

That fits our notations with

$$K(y, x-y) = \sum_{j=1}^{M} \big[a_j(y)\delta(x-y=\varepsilon\nu_j), \qquad k(x) = \sum_{j=1}^{M} a_j(x).$$

The reaction rate equations are obtained as the hyperbolic limit. Because of the homogeneity of Dirac masses, this only requires that $a_j = O(\frac{1}{\varepsilon})$ (a choice of time scale). Then we obtain, applying the results of Sect. 9.7,

$$\frac{\partial}{\partial t} p(t,x) + \operatorname{div}[Up] = 0, \qquad U_i = \sum_{j=1}^{M} \nu_{ji} a_j(x), \quad x \in \mathbb{R}^N.$$

According to the method in Sect. 8.4, the solution is given through the characteristics

$$\frac{d}{dt} Y_i(t) = \sum_{j=1}^{M} \nu_{ji} a_j(Y(t)), \qquad i = 1, \dots, N.$$

These are the reaction rate equations introduced in Sect. 1.2.1.

In the diffusive scale one can also derive the chemical Fokker-Planck equation, similar to our derivation in Sect. 9.4, that is written

$$\frac{\partial}{\partial t} p(x,t) = \frac{1}{2} \sum_{i,\,i'=1}^{N} \frac{\partial^2}{\partial x_i \partial x_{i'}} \Big[\sum_{j=1}^{M} \nu_{ji}\nu_{ji'} a_j(x) p(x,t)\Big] - \sum_{i=1}^{N} \frac{\partial}{\partial x_i} \Big[\sum_{j=1}^{M} \nu_{ji} a_j(x) p(x,t)\Big].$$

Because $\nu = O(\varepsilon)$, one can think of it as a first order expansion in the parameter ε because the diffusion matrix is of the order of $O(\varepsilon)$ compared to the transport term.

Notice the desirable properties of the matrix

$$B_{i,i'}(x) = \sum_{j=1}^{M} \nu_{ji}\nu_{ji'}a_j(x)$$

which is symmetric and nonnegative.

References

1. Gillespie, D.T.: The chemical Langevin and Fokker-Planck equations for the reversible isomerization reaction. J. Phys. Chem. A **106**, 5063–5071 (2002)
2. Perthame, B.: Transport Equations Arising in Biology. L. N. series ‘Frontiers in Mathematics’. Birkhauser, Basel (2007)
3. Stevens, A.: Derivation of chemotaxis-equations as limit dynamic of moderately interacting stochastic many particle systems. SIAM J. Appl. Math. **61**, 183–212 (2000)

Chapter 10
Fast Reactions and the Stefan Free Boundary Problem

Departing from reaction-diffusion systems one can rescale the problem and consider the global length (experimental, computational, observation) of the domain rather than the intuitive scale which, e.g. in population biology, is the individual size scale. By doing so, we rescale the space variable and this leads us to also rescale time. This allows us to use the propagation time scale rather than the generation scale.

There are many different ways to change scale (see for example Sects. 5.3.1, 9.6) and we shall only discuss the fast reaction scale. This can also be seen as a space-time *parabolic scale* where the old time is defined as $\tilde{t} = \frac{t}{\varepsilon}$, with t the new time. Then we also replace the old space variable $\tilde{x}$ by x, with the relation $\tilde{x} = \frac{x}{\sqrt{\varepsilon}}$ so as to keep the diffusion ratio $x/\sqrt{t}$ unchanged.

Depending on the type of reaction terms, the resulting asymptotic can be different. Here we consider two examples of limits describing phase transitions, namely the Stefan problem with or without latent heat.

10.1 Derivation of the Stefan Problem (No Latent Heat)

We borrow our first example from D. Hilhorst et al. [5]. We consider the reaction-diffusion equation

$$\begin{cases} \frac{\partial}{\partial t} u_\varepsilon - d_1 \Delta u_\varepsilon = -\frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \qquad t \geq 0, \ x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} v_\varepsilon - d_2 \Delta v_\varepsilon = -\frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \\ u_\varepsilon(t=0,x) = u_\varepsilon^0(x) \geq 0, \qquad v_\varepsilon(t=0,x) = v_\varepsilon^0(x) \geq 0, \qquad u_\varepsilon^0, \ v_\varepsilon^0 \in L^\infty \cap L^1(\mathbb{R}^d). \end{cases} \tag{10.1}$$

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1_10

For existence, It is easy to adapt the method of Sect. 3.10 and prove that there is a unique nonnegative solution to (10.1).

Our purpose is to establish the connection to the Stefan problem without latent heat, one formulation of which is

$$\frac{\partial}{\partial t}w - \Delta A(w) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \tag{10.2}$$

with

$$A(w) = \begin{cases} d_2 w & \text{for } w \leq 0, \\ d_1 w & \text{for } w \geq 0. \end{cases} \tag{10.3}$$

Figure 10.1 shows the function $A(\cdot)$ together with the case with latent heat for comparison. This nonlinearity singularizes the hypersurface $\{u(t) = 0\}$ as a free boundary. Equation (10.2) is closely related to the porous media equation [8], which corresponds to the nonlinearity $\tilde{A}(u) = u^p$.

First of all we begin with uniform bounds. Because the right hand sides are nonpositive, we can apply the maximum principle and also integrate to obtain L^1 bounds. For all $t \geq 0$ we have

$$0 \leq u_\varepsilon(t,x) \leq \|u_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)}, \qquad 0 \leq v_\varepsilon(t,x) \leq \|v_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)}, \tag{10.4}$$

$$\begin{cases} \displaystyle\int_{\mathbb{R}^d} u_\varepsilon(t,x)dx + \int_0^t \int_{\mathbb{R}^d} \frac{u_\varepsilon(s,x)v_\varepsilon(s,x)}{\varepsilon} dxds \leq \int_{\mathbb{R}^d} u_\varepsilon^0(x)dx, \\ \displaystyle\int_{\mathbb{R}^d} v_\varepsilon(t,x)dx + \int_0^t \int_{\mathbb{R}^d} \frac{u_\varepsilon(s,x)v_\varepsilon(s,x)}{\varepsilon} dxds \leq \int_{\mathbb{R}^d} v_\varepsilon^0(x)dx. \end{cases} \tag{10.5}$$

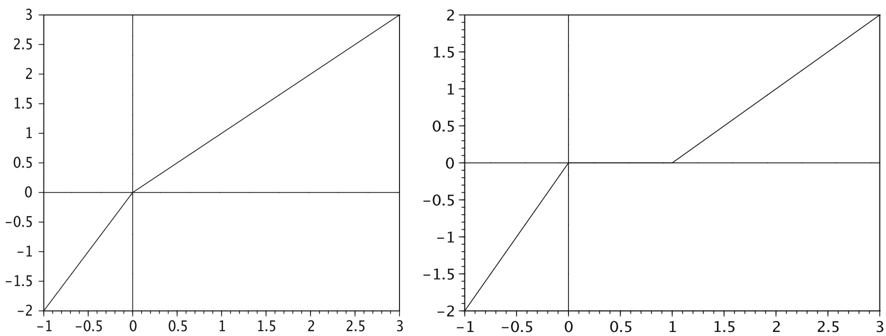

Fig. 10.1 The nonlinear diffusions in Stefan problems. *Left*: no latent heat, the function $A(\cdot)$ is according to (10.2), (10.3). *Right*: with latent heat $\lambda = 1$ here, the function $B(\cdot)$ is according to (10.13), (10.14) with $\lambda = 1$

These bounds are already a significant piece of information because they tell us that $u_\varepsilon v_\varepsilon$ should vanish as ε tends to 0. In the limit, at each point (t, x), we should have either $u(t, x) = 0$ or $v(t, x) = 0$. This is the segregation property, see also Sect. 5.3.4.

To go further, we follow the approach in M. Belhadj et al. [1]. We can obtain stronger uniform bounds, in Total Variation (TV). To do so, we assume

$$\|u_\varepsilon^0\|_{L^1(\mathbb{R}^d)} + \|u_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)} + \|v_\varepsilon^0\|_{L^1 y(\mathbb{R}^d)} + \|v_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)} \le C^0, \tag{10.6}$$

$$\|\nabla u_\varepsilon^0\|_{L^1(\mathbb{R}^d)} + \|\nabla v_\varepsilon^0\|_{L^1(\mathbb{R}^d)} \le C^1, \tag{10.7}$$

and we say that initial data are *well prepared* if

$$\left\| d_1 \Delta u_\varepsilon^0 - \frac{u_\varepsilon^0 v_\varepsilon^0}{\varepsilon} \right\|_{L^1(\mathbb{R}^d)} + \left\| d_2 \Delta v_\varepsilon^0 - \frac{u_\varepsilon^0 v_\varepsilon^0}{\varepsilon} \right\|_{L^1(\mathbb{R}^d)} \le C^2. \tag{10.8}$$

This is to say that we control initially the time derivatives.

Then, we obtain the

Theorem 10.1 (Uniform Estimates) *Consider Eq.* (10.1) *with assumptions* (10.6)–(10.8)*. Then, additional to the a priori bounds* (10.4) *and* (10.5)*, we have for all $t \ge 0$,*

$$\|\nabla u_\varepsilon(t)\|_{L^1(\mathbb{R}^d)} + \|\nabla v_\varepsilon(t)\|_{L^1(\mathbb{R}^d)} \le \|\nabla u_\varepsilon^0\|_{L^1(\mathbb{R}^d)} + \|\nabla v_\varepsilon^0\|_{L^1(\mathbb{R}^d)} := C^1,$$

$$\|\frac{\partial u_\varepsilon(t)}{\partial t}\|_{L^1(\mathbb{R}^d)} + \|\frac{\partial v_\varepsilon(t)}{\partial t}\|_{L^1(\mathbb{R}^d)} \le C^2.$$

$$u_\varepsilon \to u, \qquad v_\varepsilon \to v \qquad \textit{strongly in } L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^d),$$

$$u,\ v \in L^\infty\big(\mathbb{R}^+; L^1 \cap L^\infty(\mathbb{R}^d)\big), \qquad u(t,x)\ v(t,x) = 0 \quad \textit{a.e.}$$

and $w = u - v$ satisfies the Stefan problem (10.2)*,* (10.3)*.*

Remark 10.2 One can avoid the assumption (10.8) that the initial data is well-prepared. Then time compactness may be derived from the Lions-Aubin lemma [7]. One simply extracts from the proof below that

$$\frac{\partial}{\partial t} u_\varepsilon = \Delta(d_1 u_\varepsilon) + r_\varepsilon(t,x), \qquad \frac{\partial}{\partial t} v_\varepsilon = \Delta(d_2 v_\varepsilon) + r_\varepsilon(t,x),$$

where the quantities $(d_1 u_\varepsilon)$ and $(d_2 v_\varepsilon)$ are compact in space and r_ε is bounded in $L^1_{t,x}$. In these conditions compactness in time follows.

Proof First Step. Derivation of the Stefan Problem We first show why the singular limit of (10.1) is described by the Stefan problem without latent heat (10.2). With the *TV* estimates stated in Theorem 10.1, the families u_ε and v_ε are locally compact in $L^1_{t,x}$ (Rellich-Kondrachov theorem). Therefore, we may extract subsequences, that we still denote u_ε and v_ε, and which converge almost everywhere to limits denoted by $u,\ v \in L^\infty(\mathbb{R}^+ \times \mathbb{R}^d)$.

From the estimate for $u_\varepsilon v_\varepsilon$ on the right hand side of (10.5), we deduce

$$u\ v = \lim_{\varepsilon\to 0} u_\varepsilon v_\varepsilon = 0. \tag{10.9}$$

Next, we define

$$w_\varepsilon = u_\varepsilon - v_\varepsilon \underset{\varepsilon\to 0}{\longrightarrow} w = u - v.$$

We write, subtracting the equations for u_ε and v_ε,

$$\frac{\partial}{\partial t} w_\varepsilon - \Delta[d_1 u_\varepsilon - d_2 v_\varepsilon] = 0.$$

Passing to the limit in the distribution sense, we find, with $A = \lim_{\varepsilon\to 0}(d_1 u_\varepsilon - d_2 v_\varepsilon)$,

$$\frac{\partial}{\partial t} w - \Delta A = 0.$$

It remains to identify $A(t,x)$. For that we argue as follows

- For $w(t,x) > 0$, then $u(t,x) > 0$, thus $v_\varepsilon(t,x) \to v(t,x) = 0$ and $u_\varepsilon(t,x) \to u > 0$, and thus

$$A(t,x) = d_1 u(t,x) = d_1 w(t,x).$$

- For $w(t,x) < 0$, then $v(t,x) < 0$, thus $u_\varepsilon(t,x) \to u(t,x) = 0$ and $v_\varepsilon(t,x) \to v < 0$, and thus

$$A(t,x) = d_2 v(t,x) = d_2 w(t,x).$$

Second Step Derivation of the TV Estimate in x It remains to show the strong convergence of u_ε and v_ε. This follows from the a priori estimates, which imply local compactness. The fact that the full sequence (and not only a subsequence) converges, follows from the uniqueness of the solution of (10.2), and thus of the limit, a fact that we do not prove here, see J. Carrillo [2].

We now prove the *TV* estimates in x. We work on the equations of (10.1) and differentiate them with respect to x_i. We multiply by the sign and obtain

$$\frac{d}{dt}\int_{\mathbb{R}^d}\left[\left|\frac{\partial}{\partial x_i}u_\varepsilon(t,x)\right| + \left|\frac{\partial}{\partial x_i}v_\varepsilon(t,x)\right|\right]dx$$
$$\leq -\int_{\mathbb{R}^d}\left[\frac{\partial}{\partial x_i}u_\varepsilon\ v_\varepsilon + u_\varepsilon\ \frac{\partial}{\partial x_i}v_\varepsilon\right]\left[\operatorname{sgn}\left(\frac{\partial}{\partial x_i}u_\varepsilon(t,x)\right) + \operatorname{sgn}\left(\frac{\partial}{\partial x_i}v_\varepsilon(t,x)\right)\right]$$

$$
\begin{aligned}
&= - \int_{\mathbb{R}^d} \Big[|\frac{\partial}{\partial x_i} u_\varepsilon(t,x)| v_\varepsilon + |\frac{\partial}{\partial x_i} v_\varepsilon(t,x)| u_\varepsilon \\
&\quad + \frac{\partial}{\partial x_i} u_\varepsilon(t,x) \mathrm{sgn}\big(\frac{\partial}{\partial x_i} v_\varepsilon\big) v_\varepsilon + \frac{\partial}{\partial x_i} v_\varepsilon(t,x) \mathrm{sgn}\big(\frac{\partial}{\partial x_i} u_\varepsilon(t,x)\big) u_\varepsilon \Big] \\
&\leq 0.
\end{aligned}
$$

this is exactly the first estimate stated in Theorem 10.1.

Third Step Derivation of the TV Estimate in t The same calculation as before, but differentiating in t, gives us

$$
\frac{d}{dt} \int_{\mathbb{R}^d} \Big[|\frac{\partial}{\partial t} u_\varepsilon(t,x)| + |\frac{\partial}{\partial t} v_\varepsilon(t,x)| \Big] dx \leq 0.
$$

Therefore, we have, using the equation at time $t = 0$,

$$
\begin{aligned}
\| \tfrac{\partial}{\partial t} u_\varepsilon(t) \|_{L^1(\mathbb{R}^d)} + \| \tfrac{\partial}{\partial t} v_\varepsilon(t) \|_{L^1(\mathbb{R}^d)} &\leq \| \tfrac{\partial}{\partial t} u_\varepsilon^0 \|_{L^1(\mathbb{R}^d)} + \| \tfrac{\partial}{\partial t} v_\varepsilon^0 \|_{L^1(\mathbb{R}^d)} \\
&= \Big\| d_1 \Delta u_\varepsilon^0 - \tfrac{u_\varepsilon^0 v_\varepsilon^0}{\varepsilon} \Big\|_{L^1(\mathbb{R}^d)} + \Big\| d_2 \Delta v_\varepsilon^0 - \tfrac{u_\varepsilon^0 v_\varepsilon^0}{\varepsilon} \Big\|_{L^1(\mathbb{R}^d)}.
\end{aligned}
$$

This proves the second estimate stated in Theorem 10.1 and concludes its proof. □

10.2 Stefan Problem with Reaction Terms

We can derive an extension of the Stefan problem without latent heat, which includes reaction terms (The stationary problem in a bounded domain was studied by E.N. Dancer and Y. Du [3]). The simplest example is

$$
\begin{cases}
\frac{\partial}{\partial t} u_\varepsilon - d_1 \Delta u_\varepsilon = f(u_\varepsilon) - \frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \qquad t \geq 0, \ x \in \mathbb{R}^d, \\
\frac{\partial}{\partial t} v_\varepsilon - d_2 \Delta v_\varepsilon = g(u_\varepsilon) - \frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \\
u_\varepsilon(t=0,x) = u^0(x) \geq 0, \qquad v_\varepsilon(t=0,x) = v^0(x) \geq 0, \qquad u^0, \ v^0 \in L^\infty \cap L^1(\mathbb{R}^d).
\end{cases}
\tag{10.10}
$$

In ecology this may represent two competing species that obey, in the absence of the other species, two independent Fisher/KPP equations. Then we obtain the reaction terms

$$
f(u) = r_1 u(K_1 - u), \qquad g(u) = r_2 u(K_2 - u).
$$

Additionally, these species are strongly competitive.

The singular limit of (10.1) is described by the Stefan problem without latent heat

$$\frac{\partial}{\partial t}w - \Delta A(w) = f(w_+) - g(w_-), \qquad t \geq 0,\ x \in \mathbb{R}^d, \tag{10.11}$$

still with the definitions $w = \lim_{\varepsilon \to 0}(u_\varepsilon - v_\varepsilon)$ and $A(\cdot)$ still given by the expression in (10.3).

The derivation of this system follows exactly the same steps as the simpler case treated before in Sect. 10.1.

10.3 The Stefan Problem with Latent Heat

In order to include latent heat in the Stefan problem, the reaction-diffusion system (10.1) can be extended with a third equation. Following D. Hilhorst et al. [6], we consider the semilinear system

$$\begin{cases} \frac{\partial}{\partial t}u_\varepsilon - d_1\Delta u_\varepsilon = -\frac{1}{\varepsilon}u_\varepsilon\big[v_\varepsilon + \lambda(1-p_\varepsilon)\big], \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t}v_\varepsilon - d_2\Delta v_\varepsilon = -\frac{1}{\varepsilon}v_\varepsilon(u_\varepsilon + \lambda p_\varepsilon), \\ \frac{\partial}{\partial t}p_\varepsilon = \frac{1}{\varepsilon}\big[(1-p_\varepsilon)u_\varepsilon - v_\varepsilon p_\varepsilon\big], \end{cases} \tag{10.12}$$

and we give initial data satisfying (with uniform upper bounds in ε)

$$0 \leq u_\varepsilon^0 \leq \|u_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)}, \qquad 0 \leq v_\varepsilon^0 \leq \|v_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)}, \qquad 0 \leq p_\varepsilon^0 \leq 1.$$

The quantity $\lambda > 0$ is called the *latent heat*.

Existence and Bounds The invariant region for this system follows from the maximum principle

Lemma 10.3 *There is a weak solution of* (10.12) *satisfying for all times*

$$0 \leq u_\varepsilon(t) \leq \|u_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)}, \qquad 0 \leq v_\varepsilon(t) \leq \|v_\varepsilon^0\|_{L^\infty(\mathbb{R}^d)}, \qquad 0 \leq p_\varepsilon(t) \leq 1.$$

Proof The equations for u_ε and v_ε are Lotka-Volterra equations and the first two inequalities are simple consequences of the general positivity principle in Lemma 1.1 and the construction method in Sect. 3.10.

With these positivity results, it follows that

$$\frac{\partial}{\partial t}p_\varepsilon \geq -\frac{1}{\varepsilon}p_\varepsilon(u_\varepsilon + v_\varepsilon)$$

and consequently $p_\varepsilon \geq 0$. Similarly,

$$\frac{\partial}{\partial t}(p_\varepsilon - 1) \leq -\frac{1}{\varepsilon}(p_\varepsilon - 1)(u_\varepsilon + v_\varepsilon)$$

and thus $p_\varepsilon - 1 \leq 0$.

Then the upper bounds for $u_\varepsilon(t)$ and $v_\varepsilon(t)$ follow from the maximum principle. □

Derivation of the Equation We are going to derive the equation for the general Stefan problem with latent heat, which is written

$$\frac{\partial}{\partial t} w - \Delta B(w) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \tag{10.13}$$

with the nonlinear diffusion $B(\cdot)$ defined by

$$B(w) = \begin{cases} d_2 w & \text{for } w \leq 0, \\ 0 & \text{for } 0 \leq w \leq \lambda, \\ d_1(w-\lambda) & \text{for } w \geq \lambda. \end{cases} \tag{10.14}$$

See Fig. 10.1. Note that this is a limiting case of the unstable phase transition problem mentioned in Sect. 7.4.

The quantity w is more complicated than in Sect. 10.1. We define

$$w_\varepsilon = u_\varepsilon - v_\varepsilon + \lambda p_\varepsilon. \tag{10.15}$$

For the strong limits of u_ε, v_ε and p_ε (see the compactness estimates below), we expect to find $u \geq 0$, $v \geq 0$ and $0 \leq p \leq 1$, which cancel the right hand sides in the system (10.12). This implies the following rules

$$\begin{cases} u(t,x) > 0 \implies v + \lambda(1-p) = 0 \implies v = 0,\ p = 1 \implies w = u + \lambda, \\ v(t,x) > 0 \implies u + \lambda p = 0 \implies u = 0,\ p = 0 \implies w = -v, \\ u(t,x) = v(t,x) = 0 \implies u(1-p) - vp = 0 \implies p \in [0,1] \implies w = \lambda p. \end{cases}$$

The last line is a consequence of the first two limits and thus does not carry more information. These relations are sufficient to characterize our function w defined above as

$$w = u - v + \lambda p = \begin{cases} -v & \text{for } v > 0,\ u = 0,\ p = 0 \iff w < 0, \\ \in [0,\lambda] & \text{for } v = 0,\ u = 0,\ p \geq 0 \iff w \in [0,\lambda], \\ \lambda + u & \text{for } u > 0,\ v = 0,\ p = 1 \iff w > \lambda. \end{cases}$$

To conclude, we add up the equations of the system (10.12) (after multiplying the second line by -1 and last one by λ), we find

$$\frac{\partial}{\partial t}[u_\varepsilon - v_\varepsilon + \lambda p_\varepsilon] - \Delta[d_1 u_\varepsilon - d_2 v_\varepsilon] = 0.$$

This is also written

$$\frac{\partial}{\partial t} w_\varepsilon - \Delta[d_1 u_\varepsilon - d_2 v_\varepsilon] = 0.$$

The above relations between w and $u,\ v,\ p$ allow us to write in the limit,

$$d_1 u_\varepsilon - d_2 v_\varepsilon \underset{\varepsilon\to 0}{\longrightarrow} d_1 u - d_2 v = B(w),$$

which gives the Stefan free boundary equation with latent heat (10.14).

Strong Compactness As in the derivation of the case without latent heat, the proof of the derivation will be completed if one proves strong compactness of the families u_ε, v_ε and p_ε. This comes under the additional *TV* assumptions on the initial data

$$\|u^0_\varepsilon\|_{L^1(\mathbb{R}^d)} + \|u^0_\varepsilon\|_{L^\infty(\mathbb{R}^d)} + \|v^0_\varepsilon\|_{L^1(\mathbb{R}^d)} + \|v^0_\varepsilon\|_{L^\infty(\mathbb{R}^d)} \le C^0, \qquad 0 \le p^0_\varepsilon \le 1, \tag{10.16}$$

$$\|\nabla u^0_\varepsilon\|_{L^1(\mathbb{R}^d)} + \|\nabla v^0_\varepsilon\|_{L^1(\mathbb{R}^d)} + \|\nabla p^0_\varepsilon\|_{L^1(\mathbb{R}^d)} \le C^1, \tag{10.17}$$

and, for *TV* estimates in time we need to control initially the time derivatives and assume

$$\begin{cases} \left\| d_1 \Delta u^0_\varepsilon - \frac{1}{\varepsilon} u^0_\varepsilon \big[v^0_\varepsilon + \lambda (1 - p^0_\varepsilon \right\| \le C^2, \\ \left\| d_2 \Delta v^0_\varepsilon - \frac{1}{\varepsilon} v^0_\varepsilon (u^0_\varepsilon + \lambda p^0_\varepsilon) \right\| \le C^2, \\ \left\| \frac{\lambda}{\varepsilon} \big[(1 - p^0_\varepsilon) u^0_\varepsilon - v^0_\varepsilon p^0_\varepsilon \right\| \le C^2. \end{cases} \tag{10.18}$$

We summarize our conclusions in the following statement

Theorem 10.4 *Consider Eq.* (10.12) *with assumptions* (10.16)–(10.18)*. Then, in addition to the a priori bounds in Lemma 10.3, we have for all $t \ge 0$,*

$$\|\nabla u_\varepsilon(t)\|_{L^1(\mathbb{R}^d)} + \|\nabla v_\varepsilon(t)\|_{L^1(\mathbb{R}^d)} + \lambda \|\nabla p_\varepsilon(t)\|_{L^1(\mathbb{R}^d)}$$
$$\le \|\nabla u^0_\varepsilon\|_{L^1(\mathbb{R}^d)} + \|\nabla v^0_\varepsilon\|_{L^1(\mathbb{R}^d)} + \lambda \|\nabla^0_\varepsilon\|_{L^1(\mathbb{R}^d)} := C^1,$$

$$\|\frac{\partial u_\varepsilon(t)}{\partial t}\|_{L^1(\mathbb{R}^d)} + \|\frac{\partial v_\varepsilon(t)}{\partial t}\|_{L^1(\mathbb{R}^d)} + \lambda \|\frac{\partial p_\varepsilon(t)}{\partial t}\|_{L^1(\mathbb{R}^d)} \le 3\, C^1.$$

$$u_\varepsilon \to u, \qquad v_\varepsilon \to v, \qquad p_\varepsilon \to p \qquad \textit{strongly in } L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^d),$$

$$u,\, v,\, p \in L^\infty\big(\mathbb{R}^+; L^1 \cap L^\infty(\mathbb{R}^d)\big),$$

$$u\,\big(v + \lambda(1-p)\big) = 0, \qquad v\,\big(u + \lambda p\big) = 0, \qquad u(1-p) - vp = 0,$$

and $w = u - v + \lambda p$ *satisfies the Stefan problem with latent heat* λ (10.13), (10.14).

Proof We only prove the *TV* estimate in space; the other statements follow along the same lines as in Sect. 10.1. To simplify notations, we set $u_i = \frac{\partial u_\varepsilon}{\partial x_i}$ and drop the index ε. Once differentiated in x_i, the equations in (10.12) give

$$\begin{cases} \frac{\partial u_i}{\partial t} - d_1 \Delta u_i = -\frac{u_i}{\varepsilon}\big(v + \lambda(1-p)\big) - \frac{u}{\varepsilon}\big(v_i - \lambda p_i\big), \\ \frac{\partial v_i}{\partial t} - d_2 \Delta v_i = -\frac{v_i}{\varepsilon}\big(u + \lambda p\big) - \frac{v}{\varepsilon}\big(u_i + \lambda p_i\big), \\ \qquad\qquad \frac{\partial p_i}{\partial t} = -\frac{p_i}{\varepsilon}\big(u + v\big) + \frac{1}{\varepsilon}\big(u_i(1-p) - v_i p\big). \end{cases}$$

After multiplying each equation by the sign of the corresponding quantity according to Chap. 3, we find

$$\begin{cases} \frac{\partial |u_i|}{\partial t} - d_1 \Delta |u_i| \le -\frac{|u_i|}{\varepsilon}\big(v + \lambda(1-p)\big) + \frac{u}{\varepsilon}\big(|v_i| + \lambda |p_i|\big), \\ \frac{\partial |v_i|}{\partial t} - d_2 \Delta |v_i| \le -\frac{|v_i|}{\varepsilon}\big(u + \lambda p\big) + \frac{v}{\varepsilon}\big(|u_i| + \lambda |p_i|\big), \\ \qquad\qquad \frac{\partial |p_i|}{\partial t} \le -\frac{|p_i|}{\varepsilon}\big(u + v\big) + \frac{1}{\varepsilon}\big(|u_i|(1-p) + |v_i| p\big). \end{cases}$$

Then, the combination $|u_i| + |v_i| + \lambda |p_i|$ ensures that the positive terms of the right hand sides are compensated by the negative ones. Therefore, we find

$$\frac{\partial}{\partial t}\big[|u_i| + |v_i| + \lambda |p_i|\big] - \Delta[d_1 |u_i| + d_2 |v_i|] \le \frac{|u_i| v + u |v_i|}{\varepsilon} \le 0.$$

We conclude that

$$\frac{d}{dt} \int_{\mathbb{R}^d} \big[|u_i| + |v_i| + \lambda |p_i|\big] dx \le 0$$

and the *TV* estimate of Theorem 10.4 follows. □

10.4 The Geometric (Free Boundary) Interpretation

10.4.1 No Latent Heat

The Stefan problem has a geometric interpretation; this means that one can also describe the velocity of the free boundary $\Gamma(t)$ (the melting material) between the two phases that are determined by the sets $\Omega_-(t) = \{x \text{ s. th. } w(t,x) < 0\}$(solid phase at low temperature) and $\Omega_+(t) = \{x \text{ s. th. } w(t,x) > 0\}$(liquid phase at high temperature).

The question of regularity in the Stefan problem is not simple, see for example A. Friedmann [4]. We only argue intuitively based on the bounds in Theorem 10.1; from these we infer that for solutions of Eq. (10.2)–(10.3), $\frac{\partial w}{\partial t}$ is a bounded measure and thus also $\Delta A(w)$. This explains (at least in one dimension) that $A(w)$ is continuous, as shown in Fig. 10.2 (center). In fact, Fig. 10.2 (right) shows that $\frac{\partial}{\partial x}A(w)$ is also continuous and has a corner; therefore $\frac{\partial w}{\partial x}$ (or $\frac{\partial w}{\partial \nu}$ in higher dimensions) has a discontinuity. Interpreting (10.2)–(10.3) in the sense of distributions, at the point $X(t)$, where $w(t,X(t)) = 0$, these no-jump/jump conditions are written

$$\begin{cases} d_2 \frac{\partial w}{\partial x}(t, X(t)_-) = d_1 \frac{\partial w}{\partial x}(t, X(t)_+), \qquad \text{(no jump for } A(w)), \\ \sigma(t) := \dot{X}(t)\big[\frac{\partial w}{\partial x}(t, X(t)_+) - \frac{\partial w}{\partial x}(t, X(t)_-)\big] = \big[\frac{\partial^2}{\partial x^2}A(w)(t, X(t)_+) - \frac{\partial^2}{\partial x^2}A(w)(t, X(t)_-)\big]. \end{cases} \tag{10.19}$$

These relations determine the time dependent speed $\sigma(t)$ of the interface (Fig. 10.3).

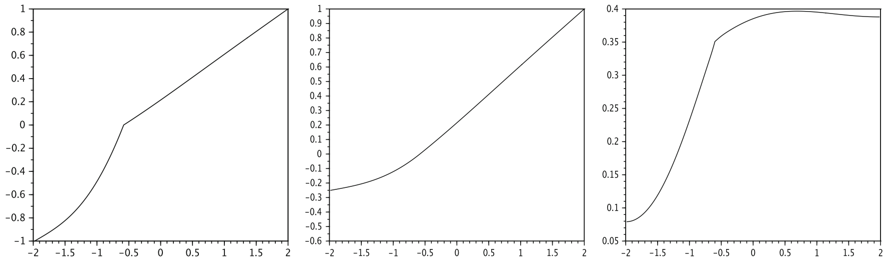

Fig. 10.2 Numerical solution of the Stefan problem (no latent heat) (10.2)–(10.3) in one dimension for $x \in (-2, 2)$ (in abscissae). *Left*: the solution $w(x)$. *Center*: the nonlinear diffusion $A\big(w(x)\big)$. *Right*: the derivative $\frac{\partial}{\partial x}A\big(w(x)\big)$

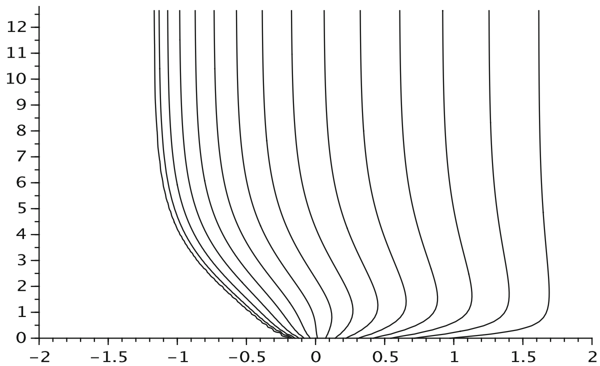

Fig. 10.3 As in Fig. 10.2 (no latent heat), we show the isolines of the phase $w > 0$. This shows the moving (with negative speed) free boundary delimitating the set $\Omega(t) := \{x; w(t,x) > 0\}$. In the abscissa is x, ordinate is time

10.4.2 With Latent Heat

When latent heat is considered, the solution of the Stefan problem (10.13)–(10.14) becomes more involved. The solid and liquid phases, which are now defined by $\Omega_-(t) = \{x \text{ s. th. } w(t,x) < 0\}$(solid phase at low temperature) and $\Omega_+(t) = \{x \text{ s. th. } w(t,x) > \lambda\}$(liquid phase at high temperature).

In addition to these phases, another state can exist. The so-called *mushy region* refers to the points

$$\Omega_m(t) = \{x \;\text{ s. th. } 0 \le w(x,t) \le \lambda\}.$$

In phase transitions, the mushy region is a phase where, in an intimate mixture (grains, dendrites), the solid and liquid phases can co-exist. Specific microscopic models are used to describe this region in detail but this is beyond the scope of this presentation. Several authors have studied circumstances of appearance and disappearance of this mushy region. It has been proved that, after some time, the mushy region disappears and this is the regime we consider here.

The geometric interpretation is then very different from (10.19) because the solution is very different, see Fig. 10.4. Again we argue in one dimension for simplicity. The points $X(t)$ of the free boundary between the two sets $\Omega_-(t)$ and $\Omega_+(t)$ are discontinuity points where w jumps form 0 to λ. Interpreting (10.13)–(10.14) in the sense of distributions, on the one hand we write the singular part as

$$\frac{\partial}{\partial t} w(t,x) = \lambda \dot{X}(t) \delta(x - X(t)) + \text{smoother}$$

because $w(t, X(t)_+) - w(t, X(t)_-) = \lambda$. On the other hand, we observe in Fig. 10.4 that $B(w(t,x))$ is continuous in x but $\frac{\partial}{\partial x} B(w)$ has a jump and thus

$$\Delta B(w) = \Big[\frac{\partial}{\partial x} B\big(w(t, X(t)_+)\big) - \frac{\partial}{\partial x} B\big(w(t, X(t)_-)\big)\Big]\, \delta(x - X(t)) + \text{smoother}.$$

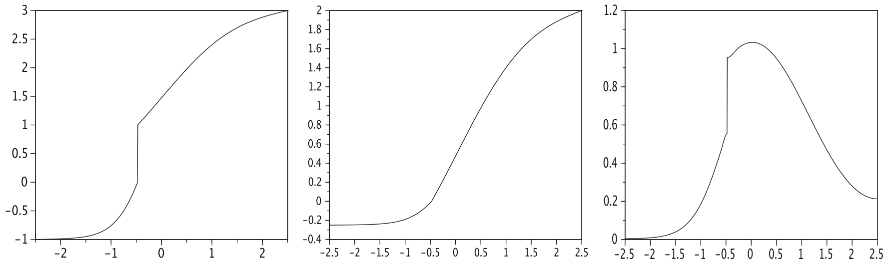

Fig. 10.4 Numerical solution of the Stefan problem with latent heat (10.13)–(10.14) in one dimension for $x \in (-2.5, 2.5)$. *Left*: the solution w. *Center*: the nonlinear diffusion $B(w)$. *Right*: the derivative $\frac{\partial}{\partial x} B(w)$

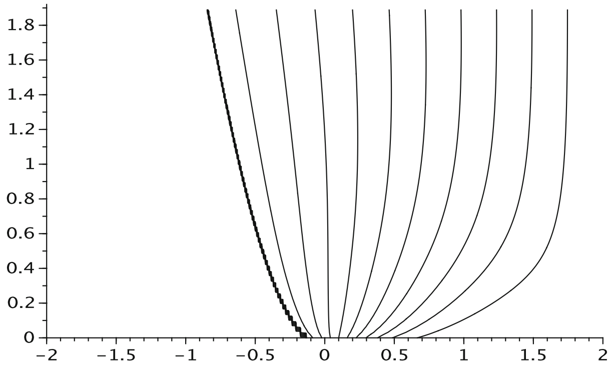

Fig. 10.5 As in Fig. 10.4, we show the isolines of the phase $w > 0$

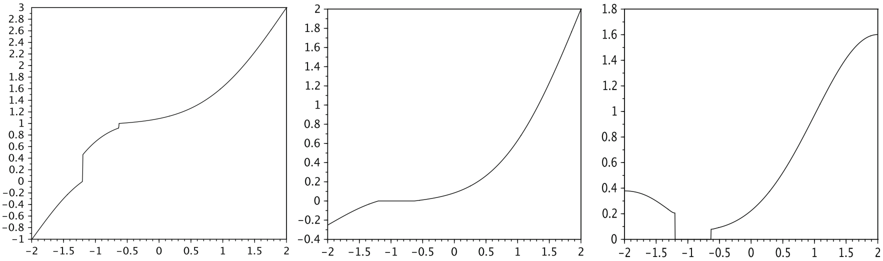

Fig. 10.6 Numerical solution of the Stefan problem with latent heat (10.13)–(10.14) in one dimension for $x \in (-2, 2)$ including a mushy region. *Left*: the solution $w(x)$. *Center*: the nonlinear diffusion $B\big(w(x)\big)$. *Right*: the derivative $\frac{\partial}{\partial x} B\big(w(x)\big)$

We arrive to the interface speed (Fig. 10.5)

$$\sigma(t) := \dot{X}(t) = \frac{d_1 \frac{\partial}{\partial x}\big(w(t, X(t)_+)\big) - d_2 \frac{\partial}{\partial x}\big(w(t, X(t)_-)\big)}{\lambda}.$$

In higher dimensions, the interface moves with a velocity proportional to the jump of normal derivatives according to the law

$$\lambda\ \sigma(t, x) = d_1 \frac{\partial w}{\partial \nu}|_{x \in \Omega_+} - d_2 \frac{\partial w}{\partial \nu}|_{x \in \Omega_-}. \tag{10.20}$$

10.4.3 Mushy Region

During a transient state, the solution contains a mushy region where $w(t, x) \in (0, \lambda)$. In Figs. 10.6 and 10.7 we show the solution. In particular, we observe that the mushy region is delimited by discontinuities of the solution w. The size of the jumps

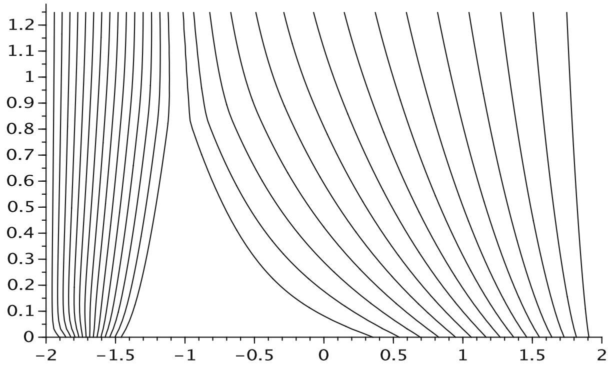

Fig. 10.7 For the Stefan problem with latent heat, the isolines of the phase $w < 0$ (isolines on the *left*) and $w > \lambda$ (isolines on the *right*). The *empty space* in between is the diminishing mushy region delimited by two discontinuities as shown in Fig. 10.6 left

increases and the mushy region diminishes and eventually disappears in finite time giving the solution of Figs. 10.4 and 10.5.

References

1. Belhadj, M.; Gerbeau J.-F., Perthame, B.: A multiscale transport model of colloids with degenerate anisotropic diffusion. Asymptot. Anal. **34**(1), 41–54 (2003)
2. Carrillo, J.: Entropy solutions for nonlinear degenerate problems. Arch. Ration. Mech. Anal. **147**(4), 269–361 (1999)
3. Dancer, E.N., Du, Y.: Competing species equations with diffusion, large interactions and jumping singularities. J. Differ. Equ. **114**, 434–475 (1994)
4. Friedman, A.: Variational Principles and Free-Boundary Problems, 2nd edn. Robert E. Krieger Publishing Co. Inc., Malabar (1988)
5. Hilhorst, D., van der Hout, R., Peletier, L.A.: Nonlinear diffusion in the presence of fast reaction. Nonlinear Anal. Ser. A Theory Methods Appl. **41**(5–6), 803–823 (2000)
6. Hilhorst, D., Mimura, M., Schätzle, R.: Vanishing latent heat limit in a Stefan-like problem arising in biology. Nonlinear Anal. Real World Appl. **4**(2), 261–285 (2003)
7. Simon, J.: Compact sets in the space $L^p(0; T; B)$. Ann. Mat. Pura Appl. **146**, 65–96 (1987)
8. Vázquez, J.L.: The Porous Medium Equation. Mathematical Theory. Oxford Mathematical Monographs. The Clarendon Press, Oxford University Press, Oxford (2007). ISBN: 978-0-19-856903-9

Index

B. Perthame, *Parabolic Equations in Biology*, Lecture Notes on Mathematical Modelling in the Life Sciences, DOI 10.1007/978-3-319-19500-1