# Growth, reaction, movement and diffusion from biology

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# Contents

# Chapter 1

# Parabolic equations in biology

As first examples, we present two general classes of equations that arise in biology: Lotak-Volterra systems and chemical reactions. These are 'reaction-drift-diffusion' equations, or in mathematical classification, semilinear equations. We try to explain what mathematical properties follow from the set up of the model: nonnegativity properties and entropy methods.

For more biologically oriented textbooks, the reader can also consult [43, 41]; for mathematical tools, many books on PDEs are available as [17, 18].

## 1.1 Lotka-Volterra systems

### 1.1.1 Movement and growth

A first class arises in the area of population biology, and ecological interactions, and is 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 instance). We assume that these species move randomly according to brownian motions with a bias according to a velocity $U_i(t,x) \in \mathbb{R}^d$ and that they have growth (meaning birth and death rates) $R_i(t,x)$. Then, the system describing the dynamics of these population densities is

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

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 wish to insist on the birth and death rates $R_i$; they depend strongly on the interactions between species and we express this fact as a nonlinearity

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

A standard family of such nonlinearities is given by the quadratic interactions

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

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 not symmetric neither non-negative. 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,

• $c_{ij} > 0$, $c_{ji} > 0$: mutualistic interaction (both species help the other and benefit from it), symbiosis (association of two species which survival depends on each other),

• $c_{ij} < 0$, $c_{ji} < 0$: direct competition (both species compete for instance for the same food),

• $c_{ii} < 0$ is usually assumed so as to represent intra-specific competition.

The quadratic aspect relates to the necessity of 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 to rather use (with $\overline{c}_{ii} = -c_{ii} > 0$)

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

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 $c_{ij} \neq 0$, it is low for trophic chain and higher for a food web (species use several foods).

The original prey-predator system of 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 proportionally to the numer of sharks ($c_{12} < 0$), while the shark population grows proportionally to the small fishes theycan eat $c_{21} > 0$). 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 to the Lotka-Volterra system (1.1) satisfy very few qualitative properties; there are no a priori conservation laws (because they contain birth and death), neither entropy properties (a concept which does not seem to relevant in ecological systems). As we will see the quadratic aspect may lead to blow-up (solutions exists only for a finite time, see chapter 6). Let us only mention that it 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 Chapter 3, but we do not need that theoretical background to show the formal manipulations leading to this result.

**Proof**. (Formal) We follow the method of Stampacchia. Set $p_i = -n_i$, we still 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 section 3.8. The difficulty stems from the 'linear' definition of weak solutions to (1.1) which do not allow for nonlinear manipulations as multiplication by $(p_i)_+$. $\square$

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

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

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

(Left to the reader; see the proof of the Lemma 1.1) in section 3.8. The idendity expresses that the total number of individuals only changes according to birth and death, motion does not count.

### 1.1.3 Monotonicity principle for competitive or cooperative systems

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

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

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

**Lemma 1.2 (Monotonicity principle)** *Consider a cooperative system. Assume that two initial data are ordered:* $0 \leq n_i^0 \leq m_i^0$, $i = 1, 2$ *and assume bounds* $n_i \leq \Gamma$, $m_i \leq \Gamma$ *and* $\mathcal{R}_i \leq \Gamma$. *Then, the weak solutions in* $C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$ *to the Lotka-Volterra system (1.1)–*(1.2) *are ordered for all times*

$$n_i(t, x) \leq m_i(t, x), \qquad \forall t \geq 0,\ x \in \mathbb{R}^d,\ i = 1,\ 2.$$

**Proof**. Substracting the two equations on $n_1$ and $m_1$, we find successively

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

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

The second line is negative from our assumption $\frac{\partial}{\partial n_1}\mathcal{R}_1 \leq 0$ and thus

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{R}^d}\frac{(n_1 - m_1)_+^2}{2} + \quad & D_1\int_{\mathbb{R}^d}|\nabla(n_1 - m_1)_+|^2 \leq \int_{\mathbb{R}^d}(n_1 - m_1)_+^2\mathcal{R}_1(n_1, n_2) \\ & + \int_{\mathbb{R}^d} m_1(n_1 - m_1)_+\big(\mathcal{R}_1(m_1, n_2) - \mathcal{R}_1(m_1, m_2)\big),\end{aligned}$$

We now use that $m_1 \geq 0$, $\frac{\partial}{\partial n_2}\mathcal{R}_1(n_1, n_2) \geq 0$ and a Lipschitz constant $L$ on $\mathcal{R}_1(n_1, n_2)$, to conclude

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

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

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

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

$$\frac{du(t)}{dt} \leq 2\Gamma(1+L)u(t).$$

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

**Exercise**. In the competitive case

$$\frac{\partial}{\partial n_2}\mathcal{R}_1(n_1, n_2) \leq 0, \qquad \frac{\partial}{\partial n_1}\mathcal{R}_2(n_1, n_2) \leq 0, \qquad \frac{\partial}{\partial n_i}\mathcal{R}_i(n_1, n_2) \leq 0.$$

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

### 1.1.4 Challenges

**Variability** There is always a big inhomogeneity in living populations. For that reason, solutions to models with fixed parameters, for movement or growth, can hardly fit with experiments or observations. They are useful for explaining qualitatively these observations but not for predicting an individual behaviour, a major problem when dealing with medical applications. A natural point of view is that these parameters are statistically distributed (see the software Monolix at http://software.monolix.org/). When modeling darwinian evolutions, the parameters are part of the model solution and mutations are seen as changes in the model coefficients.

**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 below the representation of one individual. The interpretation of such tails should be questioned carefully.

## 1.2 Reaction kinetics and entropy

When large numbers of molecules are involved in a chemical reaction, the kinetics is well described by the *reaction rate equations.* These are nonlinear equations describing the number 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 chapter **??** where we introduce the *chemical master equation* which better describes small number of reacting molecules, an important topic in cell biology.

### 1.2.1 Reaction rate equations

**General form of the equations** lead to a particular structure in the right hand sides of semi-linear parabolic equations. They are written

$$\frac{\partial}{\partial t} n_i \underbrace{- D_i \Delta n_i}_{\text{molecular diffusion}} + \underbrace{n_i \, L_i \;=\; G_i}_{\text{reaction}}, \qquad t \geq 0, \; x \in \mathbb{R}^d, \quad i = 1, 2, ..., I. \tag{1.5}$$

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 $G_i \geq 0$, depending on the $n_j$'s also, 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 size of the molecules.

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

$$L_i = \sum_{\text{reactions } p} k_{p,i} \prod_{j=1}^{I} n_j^{a_{pj}} \; n_i^{-1}, \qquad G_i = \sum_{\text{reactions } p} k'_{p,i} \prod_{j=1}^{I} n_j^{b_{pj}}. \tag{1.6}$$

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

**Nonnegativity property.** We have put in factor a term $n_i$ in front of $L_i$ to insist that this term vanishes at $n_i = 0$, the loss term $L_i$ is not singular there because the product contains $\alpha_{pi} \neq 0$ when $k_{pi} > 0$ as we will see later. For that reason, as for the Lotka-Volterra systems, the nonnegativity property holds true

**Lemma 1.3** *A weak solution to (1.5) with $G_i \geq 0$ and nonnegative initial data satisfies $n_i(t,x) \geq 0$, $\forall i = 1, 2, ..., I$.*

**Proof**. Adapt the proof of lemma 1.1.

This Lemma is useful because one simple way to argue is 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 the formula (1.6), this 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 $k = 1, ..., K$, one defines the number $N_{ki}$ of atoms $k$ in the molecule $i$. Then all reactions should preserv the number of atoms and, for all $k \in \{1, ..., K\}$, the coefficients $\alpha$, $\beta$, $k$ and $k'$ should be such that

$$\sum_{i=1}^{I} N_{ki} \left[ n_i \, L_i - G_i \right] = 0, \qquad \forall (n_i) \in \mathbb{R}^I. \tag{1.7}$$

This implies that

$$\frac{\partial}{\partial t} \sum_{i=1}^{I} N_{ki} n_i = \Delta \sum_{i=1}^{I} N_{ki} D_i n_i, \tag{1.8}$$

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

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

$$\int_{\mathbb{R}^d} \sum_{i=1}^{I} N_{ki} n_i(t,x) dx = \int_{\mathbb{R}^d} \sum_{i=1}^{I} N_{ki} n_i^0(x) dx, \qquad 1 \le k \le K. \tag{1.9}$$

Except when all the diffusion rates $D_i$'s are equal (then its main part is the heat equation), it is not easy to draw conclusions out of the equation (1.8) besides the conservation law (1.9). Very few general tools, as Michel Pierre's duality estimate, are available, see the survey [46].

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

### 1.2.2 The law of mass action

**Irreversible reaction** To begin with, consider molecular species $S_i$ undergoing the only irreversible reaction

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

with $a_i$ , $b_i \in \mathbb{N}$. Then, using the law of mass action, the equation on the number densites $n_i$ of species $i$ writes

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

From the conservation of atoms, it is impossible that for alll $i$ 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 instance, still with $a_i \neq b_i \in \mathbb{N}$, the reversible reaction

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

leads to reaction kinetics equations

$$\frac{\partial}{\partial t} n_i - D_i \Delta n_i \qquad + \quad \overbrace{a_i k_+ \prod_{j=1}^{I} n_j^{a_j}}^{\text{loss of forward reacting molecules}} \qquad + \qquad \overbrace{b_i k_- \prod_{j=1}^{I} n_j^{b_j}}^{\text{loss of backward reacting molecules}}$$
$$= \quad \underbrace{b_i k_+ \prod_{j=1}^{I} n_j^{a_j}}_{\text{gainofforwardreactionproduct}} \qquad + \qquad \underbrace{a_i k_- \prod_{j=1}^{I} n_j^{b_j}}_{\text{gainofbackwardreactionproduct}} .$$

A more handful form is

$$\frac{\partial}{\partial t} n_i - D_i \Delta n_i = (b_i - a_i) \left[ k_+ \prod_{j=1}^{I} n_j^{a_j} - k_- \prod_{j=1}^{I} n_j^{b_j} \right], \qquad i = 1, 2, ..., I. \tag{1.10}$$

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

$$S(t,x) := \sum_{i=1}^{I} n_i \big[ \ln(n_i) + \sigma_i - 1 \big], \quad \text{with} \quad \sum_{i=1}^{I} \sigma_i (a_i - b_i) = \ln k_+ - \ln k_-. \tag{1.11}$$

There are different possible choices of the constant $\sigma_i$ which can be more handful depending on the cases. With this definition one can check the

**Lemma 1.4 (Entropy property for reversible reactions)** *The entropy dissipation equality holds*

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

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

The entropy dissipation property is very important because it dictates the long time behavior of the reaction. Mathematically it is also useful for a priori estimates on 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 to the reaction-diffusion equation. This has been used recently in a series of papers by L. Desvillettes and K. Fellner[1] for estimates and relaxation properties, and by T. Goudon and A. Vasseur[2] for regularity properties.

### 1.2.3 First examples

**Isomerization.** The reversible isomerization reaction is the simplest chemical reaction. The atoms within the molecule are not changed but only their space arrangement. The reaction writes

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

This is written as

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_+ n_1 = k_- n_2, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + k_- n_2 = k_+ n_1. \end{cases} \tag{1.12}$$

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

$$S(t,x) = n_1 \big[ \ln(k_+ n_1) - 1 \big] + n_2 \big[ \ln(k_- n_2) - 1 \big], \tag{1.13}$$

and one can check the entropy dissipation relation

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

**Dioxigen dissociation.** The standard degradation reaction of dioxigen in monoxigen is usually associated with hyperbolic models for fluid flows rather than diffusion. This is because it is a very energetic reaction occuring at very high temperature (for atmosphere re-entry vehicles for instance) and with reaction rates depending critically on this temperature, see [25]. But for our purpose here, we forget these limitations and consider the dissociation rate $k_1 > 0$ of $n_1 = [O_2]$ in $n_2 = [O]$, and reversely its recombination with rate $k_- > 0$

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

[1]L. Desvillettes and K. Fellner, Entropy methods for reaction-diffusion equations: Slowly growing a-priori bounds. Rev. Mat. Iberoamericana, 24 (2) (2008), 407–431.

[2]T. Goudon and A. Vasseur, regularity analysis for systems of reaction-diffusion equations, Annales de l 'ENS, 43 (1) (2010), 117–141.

This lead to

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_+ n_1 = k_-(n_2)^2, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + 2k_-(n_2)^2 = 2k_+ n_1, \end{cases} \tag{1.14}$$

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 monoxigen are needed 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 $t \geq 0$

$$\int_{\mathbb{R}^d} \big[2n_1(t,x) + n_2(t,x)\big] dx = M := \int_{\mathbb{R}^d} \big[2n_1^0(x) + n_2^0(x)\big] dx. \tag{1.15}$$

For the simple case of the reaction (1.14), the formula (1.11) for the entropy (with $a_1 = 1$, $b_2 = 2$, $b_1 = a_2 = 0$) gives

$$S(t,x) = n_1\big[\ln(k_+ n_1) - 1\big] + n_2\big[\ln(k_-^{1/2} n_2) - 1\big]. \tag{1.16}$$

One can readily check that

**Lemma 1.5** *(Entropy inequality)*

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

**Exercise**. Deduce from (1.15) 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 (1.14), integrate the equation for $n_1$.

**Hemoglobin oxidation.** Hemoglobin $Hb$ can bind to dioxigen $O_2$ 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 neurons creates desoxyhemoglobin that can be detected by MRI and thus, indirectly, indicate the location of neural activity.

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

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

This comes with two conservations laws for the total number of molecules $Hb$ and $O_2$,

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

which imply an $L^1$ control

$$M := \int [n_1(t) + n_2(t) + n_3(t) + n_4(t)] = \int [n_1^0 + n_2^0 + n_3^0 + n_4^0].$$

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

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

From (1.11) (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 study on this system can be found in B. Andreianov and H. Labani[3].

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

$$\begin{cases} \frac{\partial}{\partial t} n_1 - D_1 \Delta n_1 + k_+ n_1 n_2 = k_- n_3 n_4, \\ \frac{\partial}{\partial t} n_2 - D_2 \Delta n_2 + k_+ n_1 n_2 = k_- n_3 n_4, \\ \frac{\partial}{\partial t} n_3 - D_3 \Delta n_3 + k_- n_3 n_4 = k_+ n_1 n_2, \\ \frac{\partial}{\partial t} n_4 - D_4 \Delta n_4 + k_- n_3 n_4 = k_+ n_1 n_2. \end{cases} \tag{1.17}$$

with the $n_i \geq 0$ 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 (1.17).

[3]B. Andreianov and H. Labani, Preconditioning operators and $L^\infty$ attractor for a class of reaction-diffusion systems. Comm. Pure Appl. Anal. To appear.

### 1.2.4 Enzymatic reactions

More representative of biology are the *enzymatic reactions*, which are usually associated with the names of Michaelis and Menten[4]. A substrate $S$ can be transformed in 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 in forming a complex $SE$ first, that can be itself dissociated in $P+E$. The complex formation reaction is supposed to be reversible but the conversion to $P+E$ is supposed irreversible, 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)

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

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 in 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 wrong if $n_E^0 = 0$. This is a fundamental observation in enzymatic reactions that a very small amount of enzymes is enough to convert the substrate into the product.

Two conservation laws hold true in these equations that help understanding the above limit,

$$\begin{cases} n_E(t) + n_C(t) = n_E^0 + n_C^0 = n_E^0, \\ n_S(t) + n_C(t) + n_P(t) = n_S^0 + n_C^0 + n_P^0 = n_S^0. \end{cases} \tag{1.18}$$

Because $n_P$ does not enter the properties of the dynamics, the system is equivalently reduced to a $2\times 2$ system

$$\begin{cases} \frac{d}{dt}n_S = k_- n_C - k_+ n_S(n_E^0 - n_C), \\ \frac{d}{dt}n_C = k_+ n_S(n_E^0 - n_C) - (k_- + k_p)n_C. \end{cases} \tag{1.19}$$

Briggs and Haldane(1925) 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 alge-

[4]Michaelis, L. and Menten, M. I., Die Kinetic der Invertinwirkung. Biochem. Z., 49, 333–369 (1913)

braically from $n_S(t)$, thus leading to a single ODE for $n_S(t)$

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

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 it in a more condensed way. Since $\overline{n_C} = \frac{k_+ \overline{n_S} n_E^0}{k_- + k_+ + k_+ \overline{n_S}}$, and after adding the two equations we find the typical enzymatic reaction kinetics equation

$$\frac{d}{dt}\overline{n_S} = -n_E^0 \, \frac{k_+ \overline{n_S}}{k_- + k_+ + k_+ \overline{n_S}} \tag{1.21}$$

In other words, the law of mass action does not apply in this limit 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 a rigorous sense and we have the

**Proposition 1.6 (Validity of Michaelis-Menten law)** *The solutions to* (1.19) *and to* (1.21) *satisfy, for $n_E^0$ small, for some constant $C(n_S^0)$ independant of $n_E^0$*

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

**Proof**. We reduce the system to a slow-fast dynamics. 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

$$\begin{cases} \frac{d}{ds}u_S^\varepsilon = k_- u_C^\varepsilon - k_+ u_S^\varepsilon(1 - u_C^\varepsilon), \qquad \varepsilon \frac{d}{ds}u_C^\varepsilon = k_+ u_S^\varepsilon(1 - u_C^\varepsilon) - (k_- + k_p)u_C^\varepsilon, \\ \frac{d}{ds}\overline{u_S} = k_- \overline{u_C} - k_+ \overline{u_S}(1 - \overline{u_C}), \qquad 0 = k_+ \overline{u_S}(1 - \overline{u_C}) - (k_- + k_p)\overline{u_C}. \end{cases} \tag{1.22}$$

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 of slow-fast dynamics [21]. We will make use of the two consequences of (1.22)

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

We have from (1.18) and $u_C^\varepsilon(t=0)=0$,

(i) $0 \le u_C^\varepsilon \le 1, \qquad 0 \le \overline{u_C} \le 1,$
(ii) $0 \le u_S^\varepsilon \le n_S^0, \qquad 0 \le \overline{u_S} \le n_S^0,$
(iii) $0 \le u_C^\varepsilon \le u^M < 1, \qquad 0 \le \overline{u_C} \le u^M < 1 \qquad$ with $u^M := \frac{k_+ n_S^0}{k_+ n_S^0 + k_- + k_p}$ independent of $\varepsilon$,
(iv) $|\frac{d}{ds} u_C^\varepsilon(s)| \le K$ 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 $|R^\varepsilon(s)| \le C\varepsilon$ for some constant.
*Hints.* (ii) $u_S^\varepsilon + u_C^\varepsilon$ decreases.
(iii) Write $\frac{d}{ds} u_C^\varepsilon \le k_+ n_S^0 (1-u_C^\varepsilon) - (k_- + k_p) u_C^\varepsilon$.
(iv) Write the equation on $z(s) = \frac{d}{ds} u_C^\varepsilon(s)$ as $\varepsilon \frac{d}{ds} z + \lambda(s) z(s) = \mu(s)$ with $\lambda > k_- + k_p$ and $\mu$ bounded.
(vi) Write $\frac{1}{2} \frac{d}{ds} R^\varepsilon(s)^2 + A R^\varepsilon(s)^2 \le \varepsilon B |R^\varepsilon(s)|$, with $A > 0$, $B > 0$ two constants.

**Beyond these principles.**
For all complex chemical reactions, the detailed description of all elementary reaction is irrealistic. 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 the mass conservation and the entropy inequality may be lost; this is a condition to get pattern formation as in the example of the CIMA reaction in section 7.6.2.

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

## 1.3 Boundary conditions

When working in a domain (connected open set with smooth enough boudary) $\Omega$, we encounter two natural types of boundary conditions. The reaction-diffusion systems (1.1) or (1.5) are completed either by

• **Dirichlet boundary conditions** $n_i = 0$ on $\partial\Omega$. This means that individuals or molecules go across the boundary and do not come again in $\Omega$. This interpretation stems from the brownian motion underlying the diffusion equation. But we can see that indeed, if we consider the conservative chemical reactions (1.5) with (1.7), 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 $\nu$ the outward normal to the boundary. But with $n_i(t,x) \geq 0$ in $\Omega$ and $n_i(t,x) = 0$ in $\partial\Omega$, we have $\frac{\partial}{\partial\nu} n_i \leq 0$, therefore the total mass diminishes

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

• **Neuman boundary conditions** $\frac{\partial}{\partial\nu} n_i = 0$ on $\partial\Omega$, still with $\nu$ the outward normal to the boundary. This means that individuals or molecules are reflected when they hit the boundary. In the computation above for (1.5) with (1.7), 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 big 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 Section 2.5 which do not hold on $\mathbb{R}^d$.

## 1.4 Brownian motion and the heat equation

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

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

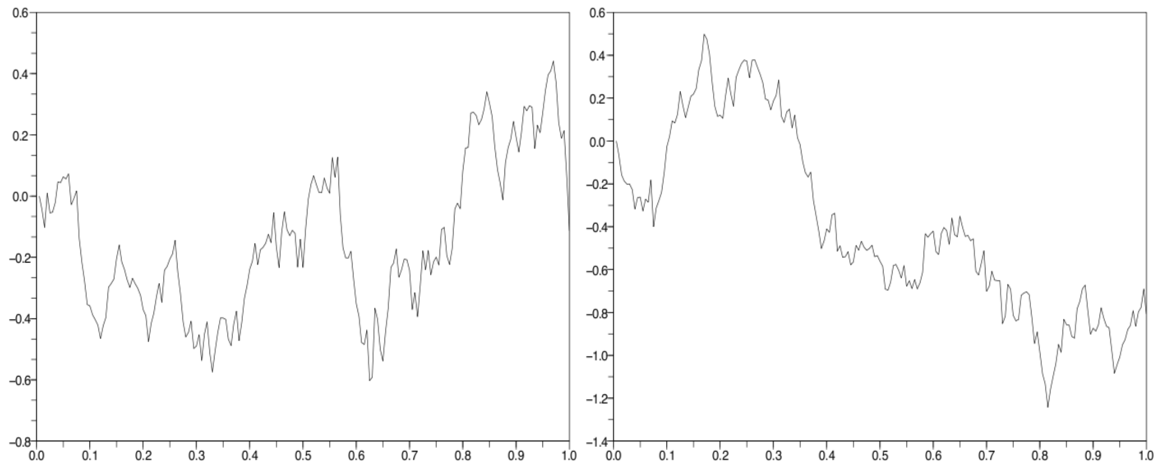


Figure 1.1: Two sample paths of the one dimensional brownian motion according to the approximation (1.23). Abscissae $t^k$, ordinates $X^k$.

On a probability space with 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

$$X^{k+1}(\omega) = X^k(\omega) + \sqrt{\Delta t}\, Y^k(\omega) \tag{1.23}$$

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

$$\mathbb{E} f(X^k, Y^k) := \int f\big(X^k(\omega), Y^k(\omega)\big) dP(\omega) = \int_{\mathbb{R}^d \times \mathbb{R}^d} f(x,y) dn^k(x)\; N(y) dy \tag{1.24}$$

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 $P\big(X^k(\omega) \in A\big) = \int_A dn^k(x)$.

Two simulations are presented. Figure 1.1 depicts, in the one dimensional case ($t^k$, $X^k$), two iterates $X^k$ (for two different $\omega$). Figure 1.2 shows two iterates $X^k$ in two dimensions.

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

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

and then

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

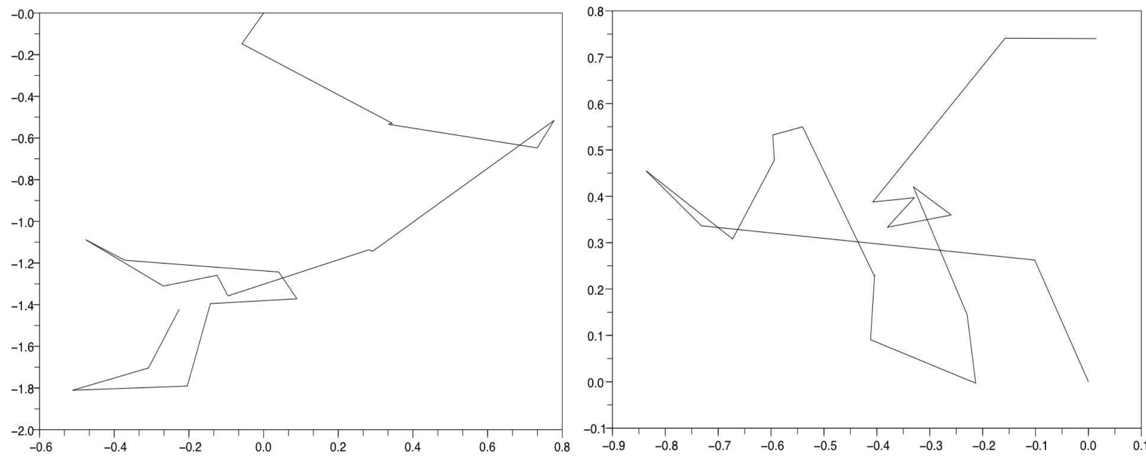


Figure 1.2: Two sample paths of the two dimensional brownian motion simulated according to (1.23).

Indeed, the formula (1.24) used with $f(x,y) = Du(X^k).Y^k$ yields, because $N(\cdot)$ is radially symmetric,

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

A further use of formula (1.24) gives

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

because $\int_{\mathbb{R}^d} y_i y_j N(y)dy = \delta_{ij}$. After dividing by $\Delta t$ and integration by parts of the term $\Delta u$, 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

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

In the distributional limit, , 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 on $n(t,x)$ (the heat equation here) is generically called the Kolmogorov equation for the limiting process (the brownian motion). Notice however that $X^k$ does not converge itself, i.e. pathwise, to the brownian motion but only in law.

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

$$n^{k+1}(x) - n^k(x) = \int \big[n^k(x + \sqrt{\Delta t}\, y) - n^k(x)\big] N(y) dy. \tag{1.25}$$

Derive the heat equation on 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 Chapter 9.

# Chapter 2

# Relaxation, perturbation and entropy methods

Solutions to nonlinear parabolic equations and systems can exhibit various and sometimes complex behaviors. This course aims at describing some of them in relation to problems arising from modeling in biology. In which circumstances can such complex behaviors 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 to parabolic equations naturally undergo regularization effects that lead them to constant or simple states. Several asymptotic results go in this direction and we present some of them in this chapter. The sections 2.1 and 2.2 have been very much influenced by the book [29].

## 2.1 Asymptotic stability by perturbation methods (Dirichlet)

The simplest possible long time 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 somehow boring and appears as the opposite of pattern formation, as e.g. when Turing instability occurs, that will be described later on, see Chapter 7.

To illustrate this, we consider, on a bounded domain $\Omega$, the semi-linear heat equation with Dirichlet boundary condition

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

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

We will use a technical result. The Laplace operator (with Dirichlet boundary condition) admits a first eigenvalue $\lambda_1 > 0$, associated with a positive eigenfuntion, $w_1(x)$, which is unique up to 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 Section 2.5 or the book [17])

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

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* $\forall u \in \mathbb{R}^I,\ t \ge 0,\ x \in \Omega,$

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

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

*then,* $u_i(t,x)$ *vanishes with exponential rate 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 $\lambda_1$, 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 by the Gronwall lemma. $\square$

**Exercise**. Consider a smooth bounded domain $\Omega \subset \mathbb{R}^d$, a real number $\lambda > 0$ and two smooth and Lipschitz continous 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 to the system

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

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 on $L$ such that for all initial data, the solution $(u,v)$ converges exponentially to $(0,0)$ for $t \to \infty$.

*Correction.* 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 easiest possible long time 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, on a bounded domain $\Omega$ with outward unit normal $\nu$, the semi-linear parabolic equation with Neumann boundary condition

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

The Laplace operator (with Neuman boundary condition) admits $\lambda_1 = 0$ as a first eigenvalue, associated with the constants $w_1(x) = 1/\sqrt{|\Omega|}$ as eigenfunction. We will use its second eigenvalue $\lambda_2$ characterized by the Poincaré-Wirtinger inequality (see [17] and Section 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

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

Notice that this is also the $L^2$ projection on the eigenspace spaned by $w_1$.

**Theorem 2.2** *(Relaxation to homogeneous solution) Assume* $\min_i D_i = d > 0$ *and*

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

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

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

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

**Proof**. Integrating in $x$ equation (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

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

Therefore, with notation (2.9)

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

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 $\partial\Omega$ (Neuman condition).
1. Prove, using the Poincaré-Wirtinger ineqality (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 on $\frac{d}{dt}\frac{\partial u_i}{\partial x_l}$.

## 2.3 Entropy and relaxation

We have seen in Lemma 1.5 that reaction kinetics equation as (1.14) are endowed with an entropy (1.16). It origins from the microscopic $N$-particles stochastic systems from which reaction kinetics are derived (at this level it is a Markov jump process which enjoys entropy dissipation as all Markov processes).

This entropy inequality is very useful also 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 Neuman boundary conditions in a bounded domain $\Omega$

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

**Theorem 2.3** *The solutions to (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*

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

*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**. 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,

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

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

$$\begin{aligned} &\textstyle\int_0^\infty \int_\Omega \ \big[D_1 \frac{|\nabla n_1|^2}{n_1} + D_2 \frac{|\nabla n_2|^2}{n_2}\big]dxdt \\ &\quad + \textstyle\int_0^\infty \int_\Omega \big[\ln(k_2\, n_2^2) - \ln(k_1\, n_1)\big]\big[k_2(n_2)^2 - k_1 n_1\big]\, dxdt \leq C(n_1^0, n_2^0). \end{aligned} \tag{2.14}$$

This is again a better 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, it says that the chemical reaction should lead the system to an equilibrium state which is space homogeneous. 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 dynamics becomes homogeneous in $x$ (but may depend on $t$). The second conclusion, combined with the mass conservation relation (1.15) 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. $\square$

**Exercise**. Consider (1.14) with Neumann boundary conditions 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 $\Sigma_1$, $\Sigma_2$ satisfy $\Sigma_1'(u) = \Sigma_2'(u^{1/2})$. Show that $\Sigma_1$ is convex if and only if $\Sigma_2$ is convex.
2. Under the conditions in question 1, show that the equation (1.14) dissipates entropy.
3. Adapt Stampacchia method to prove $L^\infty$ bounds on $n_1$, $n_2$ (and which is the natural quantity for the maximum principle). What are the natural $L^p$ bounds.

**Exercise**. Consider (1.14) with Dirichlet boundary conditions and $n_i^0 \geq 0$.
1. Using that formally $\frac{\partial n_j}{\partial \nu} \leq 0$ 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 previous exercise with the additional condition $\Sigma_i'(0) = 0$. Show that the equation (1.14) dissipates entropy.
(iii) Show that solutions to (1.14) 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 of an example that arises as a first modelling stage in two applications: 1. ecology and the model of the chemostat (the

$u$ represents a nutrient, $v$ a population that consumes the nutrient), 2. epidemiology with the celebrated Suceptible-Infected model. 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 nutrient $u$, $\mu$ the removal or degration of nutrient and $r$ the consumption rate by the population and $\mu_v$ is the mortality and removal rate of the population.

In epidemiology, $B$ represents the newborn, $\mu_u$ the mortality rate, $r$ the encounter rate between susceptibles and infected which creates new infected, $\mu_v$ is the mortality of 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 signe 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* $rB \leq \mu_u\mu_v$ *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 to the system* (2.15) *behaves 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 the system gets extinct (it converges as $t \to \infty$ to the trivial steady state).*

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 $v(t) \to 0$ and the result (ii) follows, otherwise $S$ stays bounded and converges to a finite value, (iii) conclude from 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 Dirichlet boundary condition

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

or Neuman boundary condition

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

### 2.5.1 Main results

**Theorem 2.7 (Dirichlet)** *Consider a bounded connected open set $\Omega$, then there is a spectral basis $(\lambda_k, w_k)_{k\ge1}$ for (2.19), that is,*
*(i) $\lambda_k$ is a nondecreasing sequence with $0 < \lambda_1 < \lambda_2 \le \lambda_3 \le ... \le \lambda_k \le ...$ and $\lambda_k \underset{k\to\infty}{\longrightarrow} \infty$,*
*(ii) $(\lambda_k, w_k)$ are eigenelements, i.e., for all $k \ge 1$ we have*

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

*(iii) $(w_k)_{k\ge1}$ is an orthonormal basis of $L^2(\Omega)$,*
*(iv) we have $w_1(x) > 0$ in $\Omega$ and the first eigenvalue $\lambda_1$ is simple, and for $k \ge 2$, the eigenfunction $w_k$ changes sign and maybe multiple.*

**Theorem 2.8 (Neuman)** *Consider a $C^1$ bounded connected open set $\Omega$, then there is a spectral basis $(\lambda_k, w_k)_{k\ge1}$ for (2.20), i.e.,* *(i)* $\lambda_k$ *is a nondecreasing sequence with* $0 = \lambda_1 < \lambda_2 \le \lambda_3 \le ... \le \lambda_k \le ...$ *and* $\lambda_k \underset{k\to\infty}{\longrightarrow} \infty$,

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

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

*(iii)* $(w_k)_{k\ge1}$ *is an orthonormal basis of* $L^2(\Omega)$

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

**Remark 1.** The hypothesis that $\Omega$ is connected is just used to guarantee that the first eigenvalue is simple and the corresponding eigenfunction is positive in $\Omega$. Otherwise we have several non-negative eigenfunctions with 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 conditions) and $H^1(\Omega)$ for Neuman conditions. Indeed, if $w_k$ is orthogonal to $w_j$ in $L^2(\Omega)$, then from the Laplace equation on $w_k$ and 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 $H^1$.

Notice that for $k \ge 2$, 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 matter see [49]Ch. 7, [23] Ch. 5, [9] 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 usual and is a consequence of the Krein-Rutman theorem (infinite dimension version of the Perron-Froebenius theorem).

*First step. 1st eigenelements.* On the Hilbert space $H = L^2(\Omega)$, we consider the linear subspace $V = H_0^1(\Omega)$. Then we define the minimum on $V$

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

It is attained 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 [17]). Therefore

$\int_\Omega |\nabla w_1|^2 dx \leq \liminf_{n\to\infty} \int_\Omega |\nabla u_n|^2 dx = \lambda_1$. This implies the 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 $\Omega$ (by elliptic regularity)

*Second step. Positivity.* Because in $V$, $\big|\nabla |u|\big|^2 = |\nabla u|^2$ 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 for the Laplace equation, we obtain that $w_1$ is positive inside $\Omega$ (because it is connected). This also proves that all the eigenfunctions associated with $\lambda_1$ have a sign in $\Omega$ because, on 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, a linear combination would allow to build one which changes sign (by orthogonality to $w_1$ for instance) 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

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

It is attained by the same reason as before. The variational form gives that the minimizers are solutions to the $k+1$-th eigenproblem. They can form a multidimensional space. But it is finite dimensional; otherwise we would have an infinite dimensional subspace of $L^2(\Omega)$ which unit ball is compact by 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 built (with oscillations or sharp gradients) functions satisfying $\int_\Omega |u_n|^2 = 1$ and $\int_\Omega |\nabla u_n|^2 dx \geq n$. $\square$

### 2.5.2 Rectangles: explicit solutions

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

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

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

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

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

$$w_{kl} = b_{kl} \cos\big((k-1)\pi \frac{x}{L_1}\big) \cos\big((l-1)\pi \frac{x}{L_2}\big), \quad \lambda_{kl} = \big((\frac{k-1}{L_1})^2 + (\frac{l-1}{L_2})^2\big)\pi^2, \qquad \text{(Neuman)}$$

These examples indicate that

• The first positive eigenvalue is of order $1/\max(L_1, L_2)^2 = \frac{1}{\operatorname{diam}(\Omega)^2}$. On a large domain (even with a large aspect ratio) we can expect that the first eigenvalues is close to zero and that the eigenvalues are close to each other.

• Except the firstone, eigenvalues can be multiple (take $L_1/L_2 \in \mathbb{N}$).

• Large eigenvalues are associated with highly oscillating eigenfunctions.

### 2.5.3 The numerical artefact

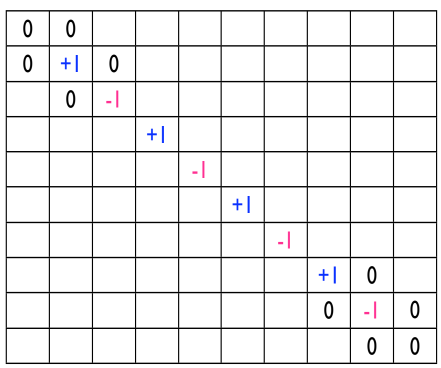


Figure 2.1: A parasite discrete eigenfunction of Laplace equation in 2 dimensions associated with the eigenvalue $\frac{2}{\Delta x^2}$. This does not approximate a continuous eigenfunction.

The numerical computation of the high eigenvalues is a difficult question. Indeed, the discrete eigenproblem may exhibit parasite eigenvalues that do not converge to a continuous eigenfunction in the limit. Figure 2.1 gives an example of this artefact in 2 dimensions.

## 2.6 The Lotka-Volterra prey-predator system with diffusion (Problem)

In the case the Lotka-Volterra prey-predator system we can show relaxation towards an homogeneous solution. The coefficients of the model need not be small as it is required in Theorem

2.2. This is because the model comes with a natural quantity (as the 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 the question 2., that the solutions are periodic (trajectories are closed).

**Exercise**. Let $\Omega$ a smooth bounded domain. Consider smooth positive solutions to the Lotka-Volterra equation with diffusion and Neuman 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 give 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 on the behavior of $n_i(t,x)$ as $t \to \infty$?

# Chapter 3

# Weak solutions to parabolic equations in $\mathbb{R}^d$

## 3.1 Heat equation in the full space

As a simple example of large time behavior, we consider the heat equation in the full space

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - \frac{1}{2}\Delta u(t,x) = 0, \qquad t \geq 0, \quad x \in \mathbb{R}^d, \\ u(t=0,x) = u^0(x). \end{cases} \tag{3.1}$$

Many of its properties can be sudied thanks to the representation by the fundamental solution, also called heat kernel,

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

It solves the heat equation (3.1) with initial data $u^0 = \delta$. Therefore, as we will justify in Chapter 3, the solution to (3.1) is

$$u(t,x) = K(t) * u^0 = \int_{\mathbb{R}^d} u^0(x-y)K(t,y)dy. \tag{3.2}$$

From usual properties of the convolution (in particular the various forms of the Young inequalities) we deduce the

**Theorem 3.1** *For $u^0 \in L^1(\mathbb{R}^d)$, we have*

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

In particuler for $p = 1$ there is no decay because $p' = \infty$ and $C(1) = 1$ because

$$\int_{\mathbb{R}^d} K(t,y)dy = 1.$$

The fastest decay rate is measured in $L^\infty$ and it is $t^{-d/2}$ as the heat kernel itself.
**Proof**. We write thanks to the Young inequalities

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

It remains to compute

$$\int_{\mathbb{R}^d} K(t,y)^p dy = \frac{1}{(2\pi t)^{pd/2}} \int_{\mathbb{R}^d} e^{-\frac{p|y|^2}{2t}} dy \leq \frac{C}{t^{pd/2}} t^{d/2} = Ct^{\frac{pd}{2p'}}.$$

□

The phenomena that is behind these estimates is dipsersion. Consider $u^0 \geq 0$ and thus $u(t, x \geq 0$ (because $K(t, y > 0)$. Then we have

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

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

Having in mind individuals that 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 od the second moment of the distribution: if it grows linearly in time, this is a sign a normal diffusion and the slope gives the diffusion coefficient.

## 3.2 Weak solutions in distributions sense

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

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = f \qquad \text{in } \mathbb{R}^d, \\ u(t=0,x) = u^0(x). \end{cases} \tag{3.3}$$

According to the general theory of distributions (due to Laurent Schwartz), these are defined through a formal integration by parts on a test function

**Definition 3.2** *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) to (3.3) if we have*

$$\int_0^\infty \int_{\mathbb{R}^d} u(t,x)[-\frac{\partial \Phi}{\partial t} - \Delta \Phi] dx\, dt = \int_0^\infty \int_{\mathbb{R}^d} f(t,x)\Phi(t,x) + \int_{\mathbb{R}^d} u^0(x)\Phi(t=0,x)\, dx, \tag{3.4}$$

*for all test functions $\Phi \in \mathcal{D}\big([0,+\infty) \times \mathbb{R}^d\big)$. 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 true obviously.

Weak solutions to linear equations enjoy many properties that make the interest of this notion.

## 3.3 Stability of weak solutions

Consider a sequence of weak solutions $u_n$ of (3.3) corresponding to data $u_n^0$ and $f_n$. Assume convergence in some weak topology (for instance $L^2$, $L^1$, $M^1$ (measures))

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

Then

**Lemma 3.3** *In this situation $u$ is a weak solution to (3.3).*

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

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

but $\Phi$ being fixed, and by the very definition of weak convergence, we can pass to the limit as $n \to \infty$ and recover the relation (3.4). $\square$

## 3.4 Mass conservation and truncation

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

**Proposition 3.4** *Assume $f \in L^1([0,T] \times \mathbb{R}^d)$, $u^0(x) \in L^1(\mathbb{R}^d)$. Let $u \in L^1([0,T] \times \mathbb{R}^d)$ for all $T > 0$ be a weak solution to (3.3), 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,*

$$\frac{d}{dt}\int_{\mathbb{R}^d} u(t,x)dx = \int_{\mathbb{R}^d} f(t,x)dx. \tag{3.5}$$

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 to the heat equation with a super-exponential growth at infinity.

We leave as an exercise the derivation of the differential equality from the integrated relation.

**Proof**. **Preliminary step.** In the definition (3.3), we can use a test function $\chi_R(x) = \chi(\frac{x}{R})$ with

$$\begin{cases} \chi \in \mathcal{D}(\mathbb{R}^d), \qquad 0 \le \chi(\cdot) \le 1, \\ \chi(x) = 1 \text{ for } |x| \le 1, \qquad \chi(x) = 0 \text{ for } |x| \ge 2. \end{cases} \tag{3.6}$$

We have for any test function $\phi \in \mathcal{D}(\mathbb{R}^+)$,

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

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

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

This is the meaning of (3.5). However, because $M_u(t)$, $M_f(t)$ are simply $L^1_{\text{loc}}(\mathbb{R}^+)$ functions, we cannot derive the integral form directly immediately.

**Proof of mass balance equation.** Let $T>0$ and consider the function $\phi(t) = \mathbf{1}_{\{0\le t\le T\}}$. It is not an admissible test function but we can choose a sequence of functions $\phi_n \in \mathcal{D}(\mathbb{R})$ with $\phi_n$ decreasing in $t$ and increasing in $n$, $\phi_n(t) \le \phi(t)$ and $\phi_n(t) = 1$ on $[0, T-1/n]$ ($n$ large enough). Then we have from the above equality

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

still by the Lebesgue Dominated Convergence Theorem applied to $M_f$.

From that, we can deduce that $M_u$ is continuous (or more accurately has a continuous representant in his Lebesgue class). Indeed, choosing $\phi_n$ nicely, at each Lebesgue point $T$ of $M_u$ one can also pass to the limit in the left hand side of the above and obtain

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

This conclues the proof of (3.5) and of Proposition 3.6. $\square$

## 3.5 Regularization of weak solutions (space)

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

**Definition 3.5** *A regularizing kernel $\omega$, this is a function satisfying the properties*

$$\omega \in \mathcal{D}(\mathbb{R}^d), \qquad \omega \geq 0, \qquad \int_{\mathbb{R}^d} \omega = 1. \tag{3.7}$$

We regularize functions by convolution and set

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

For $u \in L^1(\mathbb{R}^d)$, we have $\omega * u \in C^\infty \cap L^1(\mathbb{R}^d)$.

**Proposition 3.6** *Let $\omega$ 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 to (3.3), $u \in L^1([0,T] \times \mathbb{R}^d)$ $\forall T > 0$, then $\omega * u$ belongs to $C^1\big(\mathbb{R}^+; C^2(\mathbb{R}^d)\big)$ and is a classical solution to (3.3) for a regularized right hand side $\omega(x) * f$ and initial data $\omega * u^0$.*

**Corollary 3.7** *Consequently for any $C^2$, sublinear and convex function $S : \mathbb{R} \to \mathbb{R}$, we have in the weak sense*

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

*and also*

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

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

**Proof**. *(Classical solution)* We use the test function $\Phi(t,x) = \phi(t)\omega(y-x)$ with $y \in \mathbb{R}^d$ a fixed vector and $\phi \in \mathcal{D}(\mathbb{R}^+)$ a given test function. For this choice, the definition (3.4) gives

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

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

$$\int_0^\infty [-U(t,x)\frac{\partial \phi}{\partial t} - \Delta U(t,x)\phi(t)]dt = \int_0^\infty F(t,x)\phi(t)dt + U^0(x)\phi(0).$$

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

$$-\int_0^\infty U(t)\phi'(t)dt = \int_0^\infty G(t)\phi(t)dt + U^0\phi(0),$$

for all test functions $\phi \in \mathcal{D}(\mathbb{R}^+)$. Then we first conclude that $U \in C(\mathbb{R}^+)$ with the argument at the end of the proof of Proposition 3.4 (choosing $\phi_n \to \ \mathbf{1}_{\{0\leq t\leq T\}}$) and

$$U(t,x) = \int_0^t G(s,x)ds + U^0(x).$$

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

*(Integral inequality)* The proof is more involved because this inequality is a nonlinear statement. We use the regularization argument of the first part of this proof to obtain, for any regularizing kernel $\omega_\varepsilon = \frac{1}{\varepsilon^d}\omega(\frac{x}{\varepsilon})$, that the $C^1_t C^2_x$ function $u_\varepsilon = u * \omega_\varepsilon$ satisfies

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

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

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

Because $S(u_\varepsilon) \in C\big(\mathbb{R}^+; L^1(\mathbb{R}^d)\big)$, we can use the truncation argument of Section 3.4 to integrate and find

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

As $\varepsilon \to 0$, $u_\varepsilon \to u$ strongly in $L^1\big[0,T\big] \times \mathbb{R}^d\big)$, $\forall T > 0$, and we obtain

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

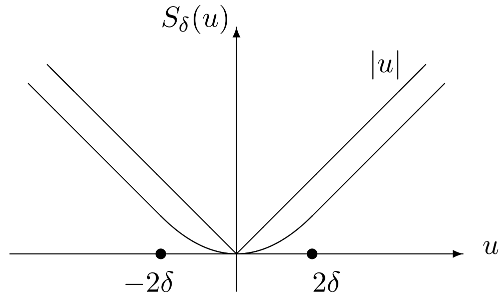


Figure 3.1: The function $S_\delta(u)$ that regularizes $|u|$.

We may finally choose a sequence $S_\delta(\cdot)$ of smooth functions as above that regularizes the absolute value. It can enjoy the properties that (see Figure 3.1 for an example):

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

Then, (3.10) gives

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

and passing to the strong limit we find the inequality 3.8. □

**Exercise**. Write and prove the same statement as Proposition 3.6 in $L^2(\mathbb{R}^d)$ in place of $L^1(\mathbb{R}^d)$ and in particular

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

## 3.6 Regularization of weak solutions (time)

We can relax the continuity assumptions in time using an additional regularization in time. To do so, there is a technical issue because $t \geq 0$ and we have to be carefull on convolution. This is the reason we introduce an asymmetric regularizing kernel $\widetilde{\omega}$, this is a function satisfying the properties

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

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

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

because we have $t - s \leq 0$ and thus for $t \geq 0$ we have $s \geq 0$.

**Theorem 3.8** *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 to (3.3), $u \in L^1\big([0,T]\times\mathbb{R}^d\big)$ $\forall T>0$, then $\big(\widetilde{\omega}(t)\omega(x)\big)*u$ belongs to $C^1\big(\mathbb{R}^+;C^2(\mathbb{R}^d)\big)$ and is a classical solution to (3.3) for a regularized right hand side $\big(\widetilde{\omega}(t)\omega(x)\big)*f$ and initial data $\omega * u^0$. Moreover*

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

We just write the main idea of the proof.

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

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

We use the test function $\Phi(s,y)=\widetilde{\omega}_\alpha(t-s)\omega(x-y)$ in the definition of weak solutions to (3.3) written with the variables $(s,y)$. Since $\widetilde{\omega}_\alpha(t)=0$ for $t\ge 0$, we find that the heat equation holds in the classical sense

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

But the initial data is not recovered and we have to use again the argument in Section 3.4 that we may use (formally) the test function in time $\phi(s)=\mathbf{1}_{\{0\le s\le t\}}$ to find

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

and thus integrating $\widetilde{\omega}(0-t)\,dt$, we find

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

With $R_\alpha(t)=\int_\infty^t\widetilde{\omega}_\alpha(s)ds$, this can be written as

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

because $0\le R_\alpha(t)\le 1$, $R_\alpha(t)\underset{\alpha\to 0}{\longrightarrow} 0$ a.e. And it follows that

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

because for $\alpha$ small enough the support of $R_\alpha$ is less than a constant $C$ and

$$|\int_0^\infty R_\alpha(-t)[\Delta(\omega*u)+\omega*f](t,x)dt| \le \int_0^C|\Delta(\omega*u)+\omega*f](t,x)|dt,$$

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

This allows us to 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 Section 3.5. $\square$

## 3.7 Uniqueness of weak solutions

A direct consequence of the regularization technique is

**Proposition 3.9** *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 $u \in L^1([0,T]\times\mathbb{R}^d)$ $\forall T>0$ to (3.3).*

**Proof**. Indeed, substracting two possible solutions $u_1$ and $u_2$, we find a solution to (3.3) 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 $u_1 = u_2$. $\square$

## 3.8 Positivity of weak solutions to Lotka-Volterra type equations

The arguments of regularization and truncation are also useful to prove the positivity of weak solutions sated 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

$$\begin{cases} \frac{\partial n}{\partial t} - \Delta n = nR(t,x) \qquad \text{in } \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{3.13}$$

Then we have

**Lemma 3.10** *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. We set $p = -n$, $p_+ = \max(0, p)$ and we have to justify the equation holds

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d}\big(p(t,x)\big)_+^2 dx + \int_{\mathbb{R}^d}\big|\nabla(p)_+\big|^2 = \int_{\mathbb{R}^d}\big(p(t,x)\big)_+^2 R \le \Gamma(t)\int_{\mathbb{R}^d}\big(p(t,x)\big)_+^2. \tag{3.14}$$

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 ($C^\infty$ in $x$ and $C^1$ in time if the $R$ are continuous in time) as shown in Section 3.5. We can also truncate using a function $\chi_\rho(\cdot)$. We obtain

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

Therefore the chain rule indeed gives

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

and thus

$$\begin{aligned}\tfrac{1}{2}\textstyle\int_{\mathbb{R}^d}\quad \big(\chi_\rho\omega_\varepsilon * p(t,x)\big)_+^2 dx &\le \textstyle\int_0^t\int_{\mathbb{R}^d}\big(\chi_\rho\omega_\varepsilon * p(s,x)\big)_+\chi_\rho\omega_\varepsilon * (p(s)\ R(s))ds\\ &+ \textstyle\int_0^t\int_{\mathbb{R}^d}\big(\chi_\rho\omega_\varepsilon * p(t,x)\big)_+^2 + 2\int_0^t\int_{\mathbb{R}^d}\big[|\nabla\chi_\rho\nabla\omega_\varepsilon * p|^2 + |\omega_\varepsilon * p\Delta\chi_\rho|^2\big]dx.\end{aligned}$$

We can now precise the choice of the truncation function. We set $\chi_\rho(x) = \chi(\frac{x}{\rho})$, with a function $\chi(\cdot)$ that satisfies

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

And we let $\rho \to \infty$, and thus $\chi_\rho \to 1$. In the above expression, the last integral vanishes because $|\nabla\chi_\rho| \le C/\rho$ and $|\Delta\chi_\rho| \le C/\rho^2$ while $\nabla\omega_\varepsilon * p$ and $\omega_\varepsilon * p$ are $L^2$ functions because $p$ is.

Therefore, we obtain using the Lebesgue Dominated Convergence Theorem

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

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

$$\begin{aligned}\tfrac{1}{2}\textstyle\int_{\mathbb{R}^d}\big(p(t,x)\big)_+^2 dx \quad &\le \textstyle\int_0^t\int_{\mathbb{R}^d}\big(p(s,x)\big)_+(p(s)\ R(s))ds + \int_0^t\int_{\mathbb{R}^d}\big(p(s,x)\big)_+^2\\ &\le \textstyle\int_0^t[\Gamma(s)+1]\int_{\mathbb{R}^d}\big(p(s,x)\big)_+^2.\end{aligned}$$

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 $p(t,x) \leq 0$ 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.

## 3.9 Positivity of weak solutions to reaction kinetics 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

$$\begin{cases} \frac{\partial n}{\partial t} - \Delta n + nR(t,x) = Q(t,x) \qquad \text{in } \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{3.15}$$

**Lemma 3.11** *Assume* $|R(t,x)| \leq \Gamma(t)$ *with* $\Gamma \in L^\infty_{\text{loc}}(\mathbb{R}^+)$ *and* $Q \in C\big(\mathbb{R}^+; L^2(\mathbb{R}^d)\big)$. *If* $Q \geq 0$ *and* $n^0 \geq 0$, *then* $n \geq 0$.

We leave the proof as an exercise.

## 3.10 Heat kernel and explicit solutions

Before solving a problem with variable coefficients as (3.15), it is usual (see [17, 48]) to look for the fundamental solution. This is to solve the PDE with the initial data a Dirac mass, for the heat equation this means

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

**Lemma 3.12** *The fundamental solution to the heat equation is given by the explicit form*

$$K(t,x) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}}. \tag{3.17}$$

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

$$\int_0^T \int_{\mathbb{R}^d} K(t,x)[-\frac{\partial \Phi}{\partial t} - \Delta\Phi] dx\, dt = \Phi(t=0, x=0). \tag{3.18}$$

Notice that

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

$$K(\varepsilon, x) \to \delta(x) \qquad \text{as } \ \varepsilon \to 0^+.$$

We give two proofs.

**Proof**. (1) For $\varepsilon > 0$ small enough, we have, by integration by parts,

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

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

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

As $\varepsilon \to 0$, we obtain (3.18) because

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

□

**Proof**. (2) This is a variant of the above proof. For $\varepsilon > 0$, $K_\varepsilon(t,x) = K(t+\varepsilon, x)$ is a solution to $\frac{\partial K_\varepsilon}{\partial t} - \Delta K_\varepsilon = 0$ for $t > 0$ (left as an exercise) with initial data $K(\varepsilon, x)$. As $\varepsilon \to 0$ we may apply the stability result of section 3.3 and we recover the result because $K(\varepsilon, x) \to \delta(x)$ as $\varepsilon \to 0^+$.
□

Another variant is to consider more generally $K_\varepsilon = K \star \omega_\varepsilon(x)$ with $\omega_\varepsilon$ a family of smooth functions that converge to a Dirac mass as $\varepsilon \to 0$ and apply the following remark.

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

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

Its solution is given by the convolution

$$u(t,x) = u^0 \star K(t) = \int_{\mathbb{R}^d} u^0(y) K(t, x-y) dy. \tag{3.19}$$

When $u^0$ is smooth with sub-exponential growth (so as to be able to integrate in the convolution formula), this is the smooth solution to the heat equation.

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 ithe solution to the heat equation and also

**Lemma 3.13**

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \leq \|u^0\|_{L^p(\mathbb{R}^d)}. \tag{3.20}$$

$$\|u(t)\|_{L^p(\mathbb{R}^d)} \leq C(d,p)\, t^{-d/(2p')}\, \|u^0\|_{L^1(\mathbb{R}^d)}, \qquad \frac{1}{p'} = 1 - \frac{1}{p}. \tag{3.21}$$

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

**Proof**. Using convolution inequalities, we have

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

which proves (3.20). And, 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

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

This gives (3.21) but with a constant $\frac{1}{p^{d/2}(2\pi)^{(p-1)d/2}}$ which is not optimal. □

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

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(t,x) \qquad \text{in } \mathbb{R}^d, \\ u(t=0,x) = 0. \end{cases} \tag{3.22}$$

It is given by the Duhamel formula

$$u(t,x) = \int_0^t \int_{\mathbb{R}^d} K(t-s, x-y) Q(s,y) dy\, ds.$$

**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 $u \in L^\infty([0,T] \times \mathbb{R}^d)$.

## 3.11 Nonlinear problems

### 3.11.1 A general result for Lipschitz nonlinearities

The most standard existence theory consists in Lipschitz continuous nonlinearities in $L^p(\mathbb{R}^d)$,

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(x, [u(t)]) \qquad \text{in } \mathbb{R}^d, \\ u(t=0,x) = u^0(x) \in L^p(\mathbb{R}^d). \end{cases} \tag{3.23}$$

We need two assumptions

$$\|Q(x,[u])\|_{L^p(\mathbb{R}^d)} \leq M_Q \|u\|_{L^p(\mathbb{R}^d)}, \tag{3.24}$$

$$\|Q(x,[u]) - Q(x,[v])\|_{L^p(\mathbb{R}^d)} \leq L_Q \|u - v\|_{L^p(\mathbb{R}^d)}. \tag{3.25}$$

**Theorem 3.14** *With the assumptions (3.24)–(3.25) and $u^0(x) \in L^p(\mathbb{R}^d)$ with $1 \leq p < \infty$, then there is a unique solution $u \in C(\mathbb{R}^+; L^p(\mathbb{R}^d))$ to (3.23).*

**Proof**. We consider a small $T$ (to be chosen later on), the Banach space $E = C\big([0,T]; L^p(\mathbb{R}^d)\big)$ into itself and the mapping $\Phi : E \to E$ defined by $u = \Phi(v)$ is the solution to the equation of the type (3.22)

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = Q(x,[v(t)]) \qquad \text{in } \mathbb{R}^d,\ 0 \leq t \leq T, \\ u(t=0,x) = u^0(x) \in L^p(\mathbb{R}^d). \end{cases} \tag{3.26}$$

Notice that $u \in E$ because of assumption (3.24). We claim that for $T$ small enough, $\Phi$ is a strong contraction because

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

Indeed from the properties of the solutions to (3.22) we have, using assumption (3.25),

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

and thus

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

Now choose $T$ such that $L_Q T = 1/2$. The Banach-Picard fixed poin theorem asserts there is a unique fixed point $u$. This is the unique solution to (3.23) on $[0,T]$.

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

### 3.11.2 Example 1.

Consider the local nonlinear problem

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

with

$$Q(0) = 0, \qquad |Q'(\cdot)| \leq L_Q. \tag{3.28}$$

**Corollary 3.15** *With assumption (3.28), there is a unique solution to (3.27) in* $C\big([0,T];L^p(\mathbb{R}^d)\big)$.

**Proof**. Indeed we can apply the Theorem 3.14 because bothe assumptions (3.24) and (3.25) are satisfied (the details are left to the reader). $\square$

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 of the fixed point in Theorem 3.14. The uniqueness of the weak solution $u$ for a given $Q(v)$ shows that the Picard iterations are the same for all $L^p$.

### 3.11.3 Example 2.

Consider now the local nonlinear problem

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = u(1-u), \\ u(t=0,x) = u^0(x) \qquad \text{with } 0 \le u^0 \le 1, \end{cases} \tag{3.29}$$

The Theorem 3.14 cannot be applied directly because $u \mapsto u(1-u)$ is not lipschitz continuous on $\mathbb{R}$. Nevertheless a small variant leads to the

**Corollary 3.16** *There is a unique solution to (3.29)* $u \in L^\infty([0,T]\times\mathbb{R}^d)$ *such that*

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

**Proof**. Define $Q(u) = u_+(1-u)_+$, this a Lipschitz continuous function and there is a solution to (3.27). Because $Q(\cdot) \ge 0$, the non-negativity result of Lemma 3.10 asserts that $u \ge 0$ and the same result for $1-u$ tells us that $1-u \ge 0$ (in fact we need a variant in $L^\infty$ in place of $L^2$).

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

Notice that, still applying the positivity result of Lemma 3.10 set in $L^\infty$, any solution should satisfy $0 \le u(t,x) \le 1$, and thus the bounded solution is unique. $\square$

# Chapter 4

# Traveling waves

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

This chapter gives several examples motivated by models from biology even though combustion waves[1] or phase transitions (Allen-Cahn equation) are among the most noticeable examples of traveling waves. Historically, in 1930 Fisher [19] gave a first model of wave propagation for a genetic advantage. But Kolmorov, Petrovski and Piskunov, [32], in 1937, gave the first mathematical analysis.

In biology, it can also be an epidemic spread as bubonic plague in Europe in the 14th century (see Figure 4.1). In neuroscience it can be calcium pulses propagating along a nerve, and their study motivated J. Evans when he introduced the now-called Evans function[2] for studying their stability. In ecology it can describe the progress of an invasive species in an uncolonized environment and experimental measurements also sustain that invasion front move with constant speed as predicted by reaction-diffusion equations. J. G. Skellam[3] reached this conclusion by fitting to a linear the square root of the area occupied by muskrats, a north america species, that escaped from a farm near Prague (see Figure 4.1).

[1] Zel'dovich, Y.B. , Frank-Kamenetskii, D.A. (1938). The theory of thermal flame propagation. Zhur. Fiz. Khim. 12, 100 (In Russian).

[2] J. Evans, Nerve axon equations 4: the stable and unstable impulse. Indiana Univ. Math. J. **24**(12), 1169–1190 (1975)

[3] J. G. Skellam, Random dispersal in theoretical populations (1951)

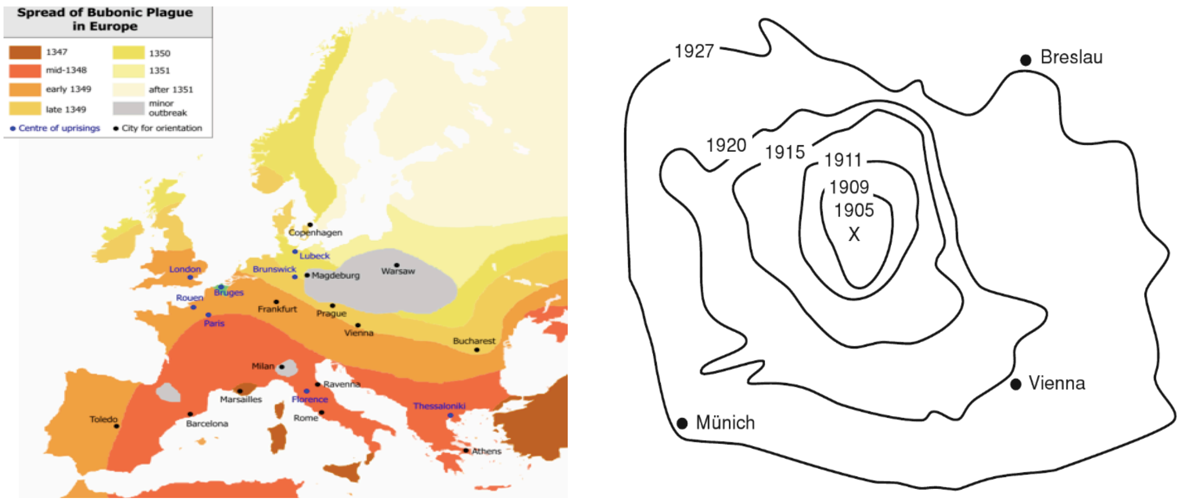


Figure 4.1: Left: propagation of plague through Europe in the middle of 14th century. Source: *http : //commons.wikimedia.org/wiki/File : Bubonic_plague_map.png*. Right: spread of muskrats in Czech Republic after J. G. Skellam and Ch. Elton.

## 4.1 Setting the problem

The simplest example is to consider the single equation

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

where $f(u)$ denotes a reaction term and $u(t,x) \in \mathbb{R}^+$ is the solution. For this type of equation we define

**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.

It is usual that $f(u)$ admits two stationary states, say $f(0) = f(1) = 0$. This is the case for instance for the so-called monostable (also called the Fisher/KPP equation) where $f(u) = u(1-u)$ or the bistable case $f(u) = u(1-u)(u-\theta)$, $0 < \theta < 1$ (also called the Allen-Cahn equation). Then, we may complete this definition with the conditions $v(-\infty) = 1$, $v(\infty) = 0$. When $c > 0$, this expresses that the state $v = 1$ invades the state $v = 0$ and vice-versa. Then we arrive to a simple equation which determines both the wave speed $c$ and the wave profile $v$

$$\begin{cases} -v''(x) - cv'(x) = f\big(v(x)\big), & x \in \mathbb{R}, \\ v(-\infty) = 1, \qquad v(+\infty) = 0. \end{cases} \tag{4.1}$$

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

There are two useful general observations. The first consists in integrating on 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

$$c = \int_{-\infty}^{\infty} f\big(v(x)\big) dx. \tag{4.2}$$

The second observation consists in computing 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

$$c \int_{-\infty}^{\infty} v'(x)^2 dx = F(1) = \int_0^1 f(v) dv. \tag{4.3}$$

For instance in the monostable case, for solutions such that $0 < v(x) < 1$, $f(\cdot) \geq 0$ and both equalities tell us that $c > 0$. This means that the state $v = 1$ is indeed invading. For the bistable case, we conclude from (4.3) that the sign of $c$ depends on the value $\theta$.

**Exercise**. Show the additional relation

$$\int_{-\infty}^{\infty} v'(x)^2 dx = \int_0^1 \big(v(x) - \frac{1}{2}\big) f(v) dv.$$

A natural question is to know what properties of the steady state make that one can connect them by a traveling wave. Many examples are treated in the litterature 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,

• 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 Chapter 7) and they can be connected by an unstable traveling wave. The example of nonlocal Fisher/KPP equation is treated in section 7.4. See also [7, 42],

• the state 0 is connected to itself by a special traveling wave called a *pulse* (homoclinic orbits), this is possible typical of the FitzHugh-Nagumo and Hodgkin-Huxley systems (electric pulse propagation along the axon).

We first give the simplest results when there is a unique pair $(c^*, v)$ that satisfies this equation (Fisher/KPP equation with ignition temperature, bistable). Then we turn to the 'unusual' case of the monostable equation where there is an infinity of traveling speeds, and finally we treat systems.

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

## 4.2 Analytical example: the monostable equation with ignition temperature

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

$$f(u) = \begin{cases} 0 & \text{for } \ 0 \le u < \theta, \\ \mu(1-u) & \text{for } \ \theta < u \le 1. \end{cases} \tag{4.4}$$

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

**Lemma 4.2** *For $f$ given by* (4.4)*, there is a unique solution $(c^*, v)$ to* (4.1) *with $v$ decreasing and normalized with $v(0) = \theta$.*

**Proof**. We know from (4.2), (4.3) that $c$ should be positive. Thanks to the normalization, 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 $w$ a linear combination of two exponential functions. Hence, we just need to consider the characteristic polynomial, that is $\lambda^2 + c\lambda - \mu = 0$. It admits two roots of which only one is positive. Therefore its solution decaying to zero at $-\infty$ is given by

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

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

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

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 $\theta$), 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. $\square$

**Exercise**. Prove that the solution $v \in (0,1)$ is unique (and thus decreasing).

## 4.3 Analytical example: the 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

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

**Lemma 4.3** *For $f$ given by (4.5), there is a unique solution $(c^*, v)$ to (4.1) with $v$ decreasing and normalized with $v(0) = \theta$.*

**Proof**. Again we may compute the unique solutions of the linear equations on $(-\infty, 0)$ 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 decaying to 0 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 the $\lambda_{r,l}$ are opposite infinity. This shows there is a unique $c$ that makes the equality.
$\square$

**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

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

**Lemma 4.4** *For $f$ given by (4.6), there is a minimal speed $c^* = 2\sqrt{1-\theta}$ and for all $c \ge c^*$ a unique solution $(c,v)$ to (4.1) normalized with $v(0)=\theta$ 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 $e^{\lambda_- x}$).*

The situation is therefore 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

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

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

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

Notice 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, expliciting the various expressions, our result is reduced to checking that

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

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

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

For $c = c^*$ see the exercise below. $\square$

**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

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

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

$$\begin{cases} -v''(x) - cv'(x) = f\big(v(x)\big), & x \in \mathbb{R}, \\ v(-\infty) = 1, \qquad v(+\infty) = 0, \qquad v(0) = \theta. \end{cases} \tag{4.8}$$

We always assume that $c > 2\sqrt{\nu}$.
1. Give the expression of $v$ for $x < 0$.
2. Give the the one parameter family of decreasing solutions for $x > 0$ and indicate the condition on 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 to find 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 $\nu$ large enough, 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 $\nu$ 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 $\nu$ is small, and thus there is an interesting question to understand the general rule for this minimal speed.

## 4.5 Analytical solutions: Problem (Non Local Fisher)

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

$$\begin{cases} -u''(x) - cu'(x) = \begin{cases} 0 & \text{for } 0 \le u < \theta, \\ 1 - K * u & \text{for } \theta < u. \end{cases}, \qquad x \in \mathbb{R}, \\ u(-\infty) = 1, \qquad u(+\infty) = 0, \qquad u(0) = \theta. \end{cases} \tag{4.9}$$

For $x<0$, we look for a complex solution $\mathbf{u}(x) = 1 - (1-\theta)e^{(\lambda + i\mu)x}$ 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 $\mathbf{u}(\mathbf{x})$ at $x = 0$.
5. What can we conclude on the problem (4.9)? Is this result usual?

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

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

Also the support of $K$ makes that makes that $x - y > 0$, that is $y < x$ and therefore the above problem is self-contained (it does not use $u(x)$ for$x > 0$). It remains to notice 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 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 $\lambda$ are positive and this is impossible.
3. $u = \theta e^{-cx} < \theta$ is the only solution to $-u'' - cu' = 0$ with $u(0) = \theta$ and $u(\infty) = 0$.
4. With 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 $\lambda$ and thus a single $c$.

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

## 4.6 The monostable equation with ignition temperature

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

$$\frac{\partial}{\partial t}u - \frac{\partial^2}{\partial x^2}u = f(u), \qquad t \geq 0,\ x \in \mathbb{R}. \tag{4.10}$$

with a reaction term given by

$$f_\theta(u) = \begin{cases} 0 & \text{for } 0 \leq u \leq \theta, \\ > 0 & \text{for } \theta < u < 1, \end{cases} \qquad f(1) = 0. \tag{4.11}$$

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

$$\begin{cases} -v''(x) - cv'(x) = f\big(v(x)\big), & x \in \mathbb{R}, \\ v(-\infty) = 1, \qquad v(+\infty) = 0. \end{cases} \tag{4.12}$$

We are going to prove the

**Theorem 4.5** *For the Fisher/KPP equation with ignition temperature, i.e., (4.10) when $f(\cdot)$ satisfies (4.11), there is a unique decreasing traveling wave solution $(c^*, v)$ normalized with $v(0) = \frac{1}{2}$ and it holds that $c^* > 0$.*

More is known about this problem, see [6, 52]. 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 natural PDE methods can be found in [6, 52].

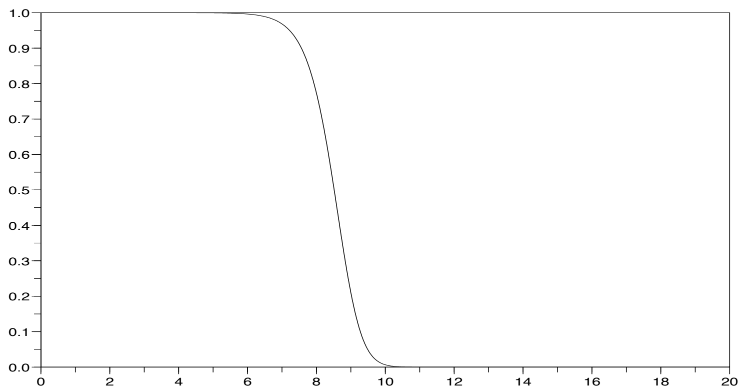


Figure 4.2: Traveling wave solution to the Fisher/KPP equation (4.28).

We decompose the proof in three steps: (i) we reduce the problem to a simpler O.D.E. (ii) we prove 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,equation (4.12) becomes a system of differential equations

$$\begin{cases} v' = -w, \\ w' = -c\, w + \ f(v), \\ v(-\infty) = 1, \ w(-\infty) = 0, \qquad v(+\infty) = 0, \ w(+\infty) = 0. \end{cases} \tag{4.13}$$

It can be further simplified because by monotonicity, we can invert $v(x)$ as a function $X(v)$, $0 \leq v \leq 1$ and define a function $\widetilde{w}(v) = w(X(v))$. In place of (4.13), we have to find a solution to

$$\begin{cases} \dfrac{d\widetilde{w}(v)}{dv} = \dfrac{dw}{dx} \, \big(\dfrac{dv}{dx}\big)^{-1} = c - \dfrac{f(v)}{\widetilde{w}}, \quad 0 \leq v \leq 1, \\ \widetilde{w}(0) = \widetilde{w}(1) = 0, \qquad \widetilde{w} \geq 0. \end{cases}$$

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

$$\begin{cases} \dfrac{d\widetilde{w}_c(v)}{dv} = c - \dfrac{f(v)}{\widetilde{w}_c(v)}, \qquad 0 \leq v \leq 1, \\ \widetilde{w}_c(0) = 0, \end{cases} \tag{4.14}$$

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

$$\widetilde{w}_c(1) = 0, \quad \widetilde{w}_c(v) \geq 0, \text{ for } \ 0 \leq v \leq 1. \tag{4.15}$$

Notice that there is a priori a singularity at $v = 0$ because the numerator and denominator vanish in the right hand side of (4.14). But for $0 \leq v \leq \theta$, $f(v) \equiv 0$ and the solution is simply

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

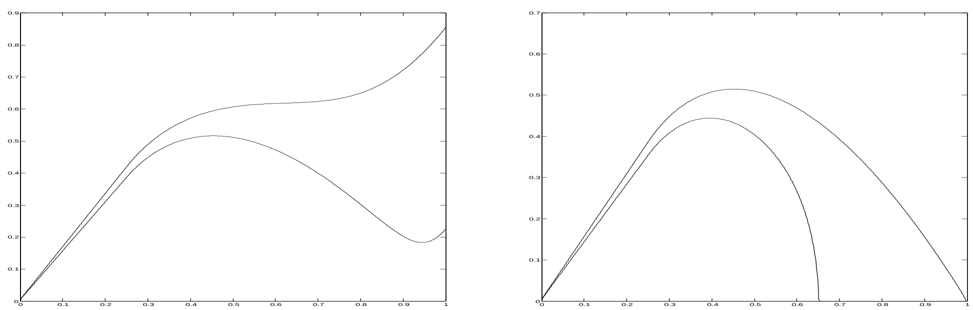

Figure 4.3: TRAVELING WAVE SOLUTIONS TO THE FISHER/KPP EQUATION WITH TEMPERATURE IGNITION (4.12) WITH THRESHOLD $\theta = .25$ PLOTED IN THE PHASE SPACE VARIABLES (4.14). WE HAVE PLOTED 4 DIFFERENT VALUES OF $c$. THE $x$-AXIS REPRESENTS $v$ AND THE $y$-AXIS REPRESENTS THE FUNCTION $\widetilde{w}(v)$. LEFT: TWO CASES WHERE THE SOLUTION TO (4.14) 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. NOTICE THAT THE $w$ SCALE IS LARGER ON THE LEFT THAN ON THE RIGHT.

Then it can be continued smoothly as a simple (nonsingular) O.D.E. untill either we reach $v = 1$, either $\widetilde{w}_c$ vanishes and the problem is not defined any longer. Numerics indicate that, depending on $c$, either we have
• $\widetilde{w}_c(v) > 0$ for $0 \leq v \leq 1$ (call it Type I), then we set $v_c = 1$, or
• $\widetilde{w}_c(v_c) = 0$ for some $0 < v_c < 1$ (call it Type II), then the equation tells us that $\widetilde{w}'_c(v_c) = -\infty$.
In both cases these are not solutions because they cannot fulfill (4.15). In the limiting case $v_{c^*} = 1$ there is a solution. These possible behaviors are depicted in Figure 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 $c \mapsto \widetilde{w}_c(v)$ is increasing for those $v$ 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*

$$\widetilde{w}_{c'}(v) \geq \widetilde{w}_c(v) + (c' - c)\, v, \qquad 0 \leq v \leq v_c. \tag{4.16}$$

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

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

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

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

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

**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*

$$\underline{c} < c^* \leq \bar{c}. \tag{4.17}$$

**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 $\widetilde{w}_c(v) \geq \frac{c}{2}v$. Because $\widetilde{w}_c(v) = c\, v$ on $[0, \theta]$ clearly $v_0 > \theta$. If $v_0 < 1$ (otherwise we are done), then $\widetilde{w}'_c(v_0) \leq \frac{c}{2}$. Then, for $\theta \leq v \leq v_0$, we have

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

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 notice that $\widetilde{w}_c(v) \leq cv$ as long as it is defined (because $\frac{f(v)}{\widetilde{w}(v)} \geq 0$) and thus

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

and thus (because the inequality is strict for $v > \theta$)

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

This implies that, if the solution did not vanish before $v = 1$, we would have $0 \leq \widetilde{w}_c(1) < c - \int_0^1 \frac{f(s)}{cs} ds$. 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 by a continuity argument on $v_c$ in the region of Type II. By the monotonicity argument of step (ii) and because of (4.16) as long as $v_c < 1$, the point $v_c$ increases continosly with controled 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 $\widetilde{w}_c(1)$ decreases uniformy 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.* $c \int_0^{v_c} \widetilde{w}_c(v)dv = \int_0^{v_c} f(v)dv$. Also use the informations in the proof to conclude that $f(v_c)\frac{dv_c}{dc} = \int_0^{v_c} \widetilde{w}_c(v)dv + c\int_0^{v_c} z_c(v)dv \geq \frac{c}{2}\theta^2 + \frac{c}{2}(v_c)^2$.

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

$$\begin{cases} \dfrac{dw}{dv} = c - \dfrac{f(v)}{\sqrt{\varepsilon^2 + w(v)^2}}, \qquad 0 \leq v \leq 1, \\ w(0) = 0. \end{cases} \tag{4.18}$$

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

**Correction** (i) Indeed, this implies $w'(1) \geq 1$ but the equation implies that $w'(1) = c > 0$.
(ii) Same proof as above.
(iii) 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 monotinicity, there is a larger $c = c^\varepsilon$ such that $w$ vanishes at some point, $w(v_\varepsilon) = 0$ and $w(v) \geq 0$. There fore we have $w'(v_\varepsilon) = 0$, which implies $\varepsilon c^\varepsilon = f(v_\varepsilon)$.
(iv) As $\varepsilon$ decreases to 0, one can check (still by monotonicity) that $c^\varepsilon$ increases to a limit $c_f > c_*$. On the otherhand, by the previous question, $f(v_\varepsilon) \to 0$. One checks that $v_\varepsilon$ remains far from $[0, \theta]$ and thus, by the assumption on $f$, we have $v_\varepsilon \to 1$. In the limit we obtain a solution to (4.14) which vanishes at $v = 1$.

## 4.7 Allen-Cahn (bistable) equation

Uniquely defined traveling waves 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

$$0 < \theta < 1. \tag{4.19}$$

It 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 $0 \le u^0 \le 1$ is invariant with time.

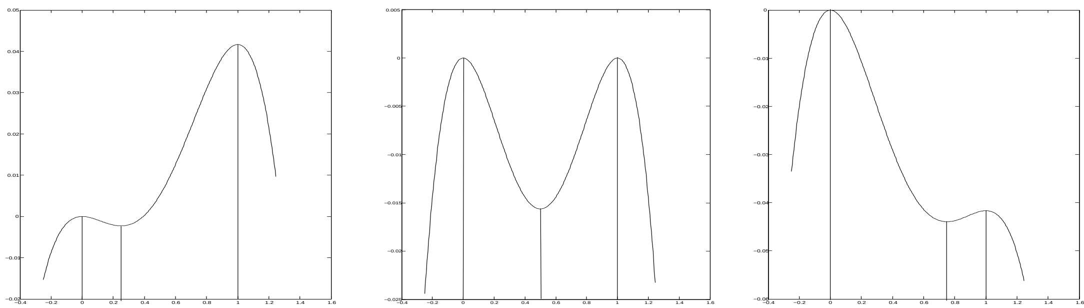

Figure 4.4: THE FUNCTION $W(u) = \int_0^u v(1-v)(v-\theta)dv$ FOR DIFFERENT VALUES OF $\theta$. LEFT: $\theta = .25$ AND $W$ IS NEGATIVE ON $(0, \beta)$ FRO SOME $\beta > \theta$ AND POSITIVE ON $]\beta, 1]$. CENTER: $\theta = .5$ AND $W(u)$ IS NONPOSITIVE AND VANISHES AT $u = 0$ AND $u = 1$. RIGHT: $\theta = .75$ AND $W$ IS NEGATIVE ON $(\beta, 1)$ FOR SOME $\beta < \theta$.

Compared to the Fisher/KPP equation, the bistable equation uses an improvement of the logistic growth term $u(1-u)$; it supposes that too low population densities $u(t)$, less than $\theta$, lead to extinction by lack of encounters between individuals. This is called Allee effect, [1]. It however takes his name from the theory of phase transitions[4].

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

$$\frac{\partial}{\partial t}u(t,x) - \Delta u(t,x) = u(t,x)\big(1-u(t,x)\big)\big(u(t,x)-\theta\big). \tag{4.20}$$

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

$$\begin{cases} -cv'(x) - v''(x) = v(x)\big(1-v(x)\big)\big(v(x)-\theta\big). \\ v(-\infty) = 1, \qquad v(+\infty) = 0, \qquad v(0) = \frac{1}{2}. \end{cases} \tag{4.21}$$

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 Fisher/KPP with ignition temperature

**Theorem 4.8** *There exists a unique decreasing solution $(c^*, v)$ to (4.21) and*

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

The sign follows from the general principle in Section 4.1.

[4] Allen, S. M. and Cahn, J. W. A macroscopic theory for antiphase boundary motion and its application to antiphase domain coarsening. Acta Metal. 270 (1979) 1085–1095

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 it connects the state $u(-\infty) = 1$ to $u(\infty) = 0$.
2. Check it statisfies the equation (4.21) and write the relation between $\theta$ 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 properties that there is a unique root $\theta$, $0 < \theta < 1$ such that

$$\begin{cases} f(0) = 0,\ f'(0) < 0, \qquad f(\theta) = 0, \qquad f(1) = 0,\ f'(1) < 0, \\ \\ f(u) < 0 \quad \text{for } 0 < u < \theta, \qquad\qquad f(u) > 0 \quad \text{for } \theta < u < 1. \end{cases} \tag{4.22}$$

Following again the general principle in Section 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* (4.22)*, there exists a unique traveling wave* $(c^*, v)$ *to (4.21) with* $v$ *decreasing and*

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

**Proof**. As in Section 4.6, we consider (4.21) 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 $X(v)$, $0 \leq v \leq 1$ and define a function $\widetilde{w}(v) = w(X(v))$. Following the derivation of (4.14) in the case of Fisher/KPP equation with ignition temperature, we arrive here to

$$\begin{cases} \dfrac{d\widetilde{w}(v)}{dv} = c - \dfrac{f(v)}{\widetilde{w}(v)}, \qquad 0 \leq v \leq 1, \\ \widetilde{w}(0) = \widetilde{w}(1) = 0, \qquad\qquad \widetilde{w} \geq 0. \end{cases} \tag{4.23}$$

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) Firstly the singularity of the right hand side at $v = 0$ can be handled with L'hospital rule and computing from (4.23)

$$\widetilde{w}'(0) - \frac{f'(0)}{\widetilde{w}'(0)} = c \iff \widetilde{w}'(0) = S(c),$$

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 Cauchy-Lipschitz theorem with singularities at the origin) to define a unique solution to

$$\begin{cases} \dfrac{d\widetilde{w}_c(v)}{dv} = c - \dfrac{f(v)}{\widetilde{w}_c(v)}, \\ \widetilde{w}(0) = 0, \qquad \widetilde{w}_c'(0) = S(c). \end{cases} \tag{4.24}$$

Because $f(v) \leq 0$ on $[0, \theta]$, we have $\frac{d\widetilde{w}_c(v)}{dv} \geq c$ and thus

$$\widetilde{w}_c(v) \geq cv \quad \text{on } [0, \theta].$$

Therefore, it is either defined and positive for all $0 \leq v \leq 1$, then we set $v_c = 1$ and call it Type I. Either it is defined on an interval $[0, v_c]$ with $\widetilde{w}_c(v_c) = 0$ and

$$v_c > \theta, \tag{4.25}$$

when the system reaches another singularity where $\widetilde{w}_c'(v_c) = -\infty$, and call it Type II.

(ii) The property holds

$$c \mapsto \widetilde{w}_c(v) \quad \text{is } C^1 \text{ and increasing for } \ 0 < v \leq v_c.$$

Indeed, following the Fisher/KPP case, we set $z_c(v) = \widetilde{w}_c(v)'$ and we have

$$\begin{cases} \dfrac{dz_c(v)}{dv} = 1 + z_c(v)\dfrac{f(v)}{\widetilde{w}_c(v)^2}, \\ z_c(0) = 0, \qquad z_c'(0) = S'(c) > \frac{1}{2}. \end{cases}$$

And the solution to this equation is positive close to $v = 0$, 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 $c$ large enough $\widetilde{w}_c(v)$ remains increasing on $[0, 1]$. In other words for $c$ large enough the solution is of type I.

We claim that the solution for $c \approx 0$ is of type II. Indeed, we can compute another relation because the equation reads

$$\frac{1}{2}\frac{d\,\widetilde{w}_c(v)^2}{dv} = c\widetilde{w}_c - f(v) = c\widetilde{w}_c - W'(v),$$

with $W(v) = \int_0^v f(z)dz$ depicted in Figure 4.4. We arrive at

$$\frac{1}{2}\widetilde{w}_c(v)^2 = c\int_0^v \widetilde{w}_c(z)dz - W(v). \tag{4.26}$$

For $c = 0$ this gives

$$\widetilde{w}_0(v)^2 = -2W(v).$$

Because $W(v) \leq 0$ on $[0,1]$ 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 $\beta$

$$W(\beta) = 0, \qquad 1/2 < \beta < 1.$$

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 by point (ii) and we can write from (4.26)

$$0 = c\int_0^{v_c} \widetilde{w}_c(z)dz - W(v_c), \qquad \widetilde{w}_c(v_c) = 0.$$

Differentiating in $c$, we obtain

$$0 = \int_0^{v_c} \widetilde{w}_c(z)dz + c\widetilde{w}_c(v_c)\frac{dv_c}{dc} - W'(v_c)\frac{dv_c}{dc} = \int_0^{v_c} \widetilde{w}_c(z)dz - W'(v_c)\frac{dv_c}{dc},$$

or also, recalling (4.25),

$$\frac{dv_c}{dc} = \frac{\int_0^{v_c} \widetilde{w}_c(z)dz}{f(v_c)} > 0.$$

So that we can define again $c^*$ as the maximum of the $c$ corresponding to type II. It has to satisfy $\widetilde{w}_{c^*}(v_{c^*}) = 0$. By strong monotonicity, or by (4.26), it is also the minimum of the $c$ giving solutions of type I. $\square$

## 4.8 The Fisher/KPP equation

We can now come to the more basic equation proposed by Fisher [19] for the propagation of a favorable gene in a population. It is to find a solution $u(t,x)$ to

$$\frac{\partial}{\partial t}u - \nu\frac{\partial^2}{\partial x^2}u = r\, u(1-u), \qquad t \geq 0,\ x \in \mathbb{R}, \tag{4.27}$$

with $\nu > 0$, $r > 0$ given parameters. They describe respectively the diffusion ability (due to active motion for instance as in zooplancton) and the growth rate of the population. The same equation is also called the KPP [32] equation and describes a combustion wave in a chemical reaction. It makes sense in any dimension but traveling waves are naturally one dimensional.

A simple observation is as follows: the steady state $u \equiv 0$ is unconditionally unstable. This means that any homogeneous small initial perturbation $\delta u^0$ will give an exponential growth $u \approx e^{rt}\delta u^0$. But the steady state $u \equiv 1$ is unconditionally stable; any homogeneous (at least) small initial perturbation $u^0 = 1 - \delta u^0$ 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 again look for solution $u(t,x) = v(x - ct)$. Inserting this definition in the Fisher/KPP equation (4.27), we obtain

$$\nu v''(x) + cv'(x) + rv(x)\big(1 - v(x)\big) = 0, \qquad x \in \mathbb{R}, \tag{4.28}$$

and because we want it to describe the progression of an invasion front corresponding to $u = 1$ into an uncolonized region $u = 0$, we complete the definition with the conditions at infinity

$$v(-\infty) = 1, \qquad v(+\infty) = 0, \qquad v(0) = 1/2, \tag{4.29}$$

and, again, the last condition is to fix the translational invariance.

The situation here very different from the case with ignition temperature and from the Allen-Cahn equation. A famous result[5] is the

**Theorem 4.10** *For any $c \geq c^* := 2\sqrt{\nu r}$, there is a unique (traveling wave) solution $v$, $0 \leq v(x) \leq 1$, to (4.28)–(4.29). It is monotonically decreasing.*

The quantity $c^*$ is called the *minimal propagation speed*. There are several ways to motivate that this speed $c^*$ corresponds to the most stable traveling wave; we mention one later based on perturbation of the nonlinear term by including an ignition temperature $\theta$ and letting $\theta$ vanish. It is also the type of wave that appears as the long time limit of the evolution equation with an initial data with compact support. See [6, 52].

The condition $c \geq c^*$ can be derived in 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 needed to have $\lambda > 0$, hence we should have $c \geq c^*$.

[5] Aranson D. G. and Weingerger H. F. Nonlinear diffusion in population genetics, combustion, and nerve pulse propagation. In Lecture Notes in mathematics Vol. 446 (1975), 5–49. Springer BErlin/Heidelberg

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 on $[0, 1]$ (this is the case of the Fisher/KPP term $u(1-u)$), the linearization method explained above and Theorem 4.10, remain 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 [18, 6, 52]. We just 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

$$\begin{cases} v' = -w, \\ w' = -\frac{c}{\nu}\, w + \frac{r}{\nu}\, v(1-v), \\ v(-\infty) = 1,\ w(-\infty) = 0, \qquad v(+\infty) = 0,\ w(+\infty) = 0. \end{cases} \tag{4.32}$$

It still can be further simplified because by monotonicity, we can still invert $v(x)$ as a function $X(v)$ and define a function $\widetilde{w}(v) = w(X(v))$. In place of (4.32), we have to find a solution to

$$\begin{cases} \dfrac{d\widetilde{w}(v)}{dv} = \dfrac{dw}{dx}\,\big(\dfrac{dv}{dx}\big)^{-1} = \dfrac{c}{\nu} - \dfrac{r}{\nu}\,\dfrac{v(1-v)}{\widetilde{w}}, \quad 0 \leq v \leq 1, \\ \widetilde{w}(0) = \widetilde{w}(1) = 0, \qquad \widetilde{w} \geq 0. \end{cases} \tag{4.33}$$

This differential equation still has singularitie at $v = 0$ and $v = 1$ but it is worse than what we have encountered yet. If we try to guess what is the slope $\widetilde{w}'(0)$, we find

$$\widetilde{w}'(0) = \frac{c}{\nu} - \frac{r}{\nu}\,\frac{1}{\widetilde{w}'(0)}, \qquad \widetilde{w}'(0) = \frac{1}{2\nu}[c \pm \sqrt{c^2 - 4\nu r}].$$

This only 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 (4.11). We denote the corresponding solution by $(c^*(\theta), \widetilde{w}^\theta(v))$. For a well-tuned $f_\theta$ in (4.11) 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 $\theta$. Therefore we can extract a sequence

$$\theta_n \to 0, \qquad c^*(\theta_n) \to c^{**}, \qquad 0 < c^{**} < \infty.$$

On the other hand from (4.14), we know know that $\widetilde{w}^{\theta\prime}(v) \leq c^*(\theta)$ and thus

$$0 \leq \widetilde{w}^{\theta}(v) \leq c^*(\theta)v.$$

Writing

$$-\max_{0 \leq v \leq 1} f^{\theta}(v) \leq \frac{d}{dv}\frac{\widetilde{w}^{\theta}(v)^2}{2} = c^*(\theta)\widetilde{w}^{\theta}(v) - f^{\theta}(v) \leq c^*(\theta)^2 v,$$

we conclude by the Ascoli Theorem that, still after extraction, $\widetilde{w}^{\theta}(v)^2$ converges uniformly. Therefore, still for the uniform convergence we have

$$\widetilde{w}^{\theta_n}(v) \underset{n\to\infty}{\longrightarrow} \widetilde{w}^{**}(v), \qquad 0 \leq \widetilde{w}^{**}(v) \leq c^{**}\, v.$$

It is easy to prove that $\widetilde{w}^{\theta_n}(v)$ remains uniformly positive in $(0,1)$ and, from (4.14), that $\frac{d}{dv}\widetilde{w}^{\theta_n}(v)$ also converges locally uniformly to a solution to (4.33).

It is possible to prove that this solution is the traveling wave with minimal speed but we will 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 (4.11) and prove uniform estimates in $\theta$ showing that we can extract subsequences which converge. We do that in several steps and drop the dependency upon $\theta$ in the course of calculations.

*1st step.* Uniform upper bound on $c^*(\theta) < c^* = 2$. This also uses the additional assumption $f^{\theta}(v) < f(v) = v(1-v)$ on $(0,1)$. We argue thy contradiction and assume $c := c^*(\theta) \geq c^*$. 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 $v'(x_0) = \lambda A_0 e^{-\lambda x_0}$, $v''(x_0) \leq \lambda^2 A_0 e^{-\lambda x_0}$, and thus, from equation (4.11)

$$0 = v''(x_0) + v'(x_0) + f^{\theta}(v(x_0)) < \lambda^2 - c\lambda + \frac{v^{\theta}(x_0)\big(1 - v^{\theta}(x_0)\big)}{v^{\theta}(x_0)} \leq \lambda^2 - c\lambda + 1 = 0,$$

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 (4.12) 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 $v$ equation (4.12)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

$$\frac{c^*(\theta)}{2} = \int_{-\infty}^{\infty} v^\theta(x) f^\theta\big(v^\theta(x)\big)dx - \int_{-\infty}^{\infty} \big(v^{\theta\prime}(x)\big)^2 dx. \tag{4.35}$$

Substracting (4.35) to (4.34), we obtain

$$\frac{c^*(\theta)}{2} = \int_{-\infty}^{\infty} \big(1 - v^\theta(x)\big) f^\theta\big(v^\theta(x)\big)dx + \int_{-\infty}^{\infty} \big(v^{\theta\prime}(x)\big)^2 dx > 0 \qquad \text{(uniformly in } \theta\text{)}. \tag{4.36}$$

*3rd step.* Uniform bound on $v'$. We multiply (4.12) 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 again 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 $\infty$, 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 to the equation (4.12) prove that $v''$ is uniformly bounde. Then we can pass to the uniform limits in (4.12) and find a solution to 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 does not bring new conditions on $c$ compared to (4.30).

**Exercise**. In (4.11), choose $f_\theta$ increasing in $\theta$. Set $\zeta(v) = \frac{d}{d\theta}\widetilde{w}^\theta(v)$
1. Write a differential equation on $\zeta$.
2. Since $\zeta(v) = 0$ on $[0, \theta]$, 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.
*Correction.* $\frac{d}{dv}\zeta(v) = -\frac{df_\theta(v)}{d\theta}\,\frac{1}{\widetilde{w}^\theta(v)} + \zeta(v)\frac{f_\theta(v)}{\big(\widetilde{w}^\theta(v)\big)^2}$.

## 4.9 The Diffusive Fisher/KPP system

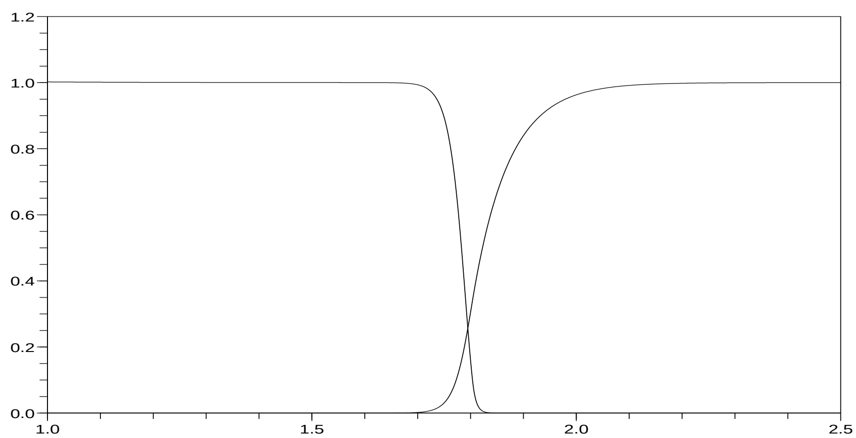


Figure 4.5: The traveling wave profile for the Diffusive Fisher equation with $d_u = 1$, $d_v = 10$ and $g(u) = u$. The first unknown $u$ has a decreasing sharp front and $v$ a wide increasing shape.

Another system related to the Fisher/KPP equation arises in modeling both combustion[6] and bacterial colonies[7] (models for bacterial colonies growth are treated in details in [26]).

[6] J. Billingham and N. L. Needham. The development of travelling waves in quadratic and cubic autocatalysis with unequal diffusion rates. I. Permanent form travelling waves. Phil. Trans. R. Soc. Lond. A (1991) 334, 1–24

[7] D. A. Kessler and H. Levine. Fluctuation induced diffusive instabilities, Nature, 394 (1998), 556–558.

The so-called *Diffusive Fisher* 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 have considered again a truncation function $g(\cdot) \in C^2([0,\infty))$, and because there is a priori no maximum principle for this system, we have to define it on the positive half-line

$$g(0) = 0, \qquad g'(0) = 0, \qquad g'(u) > 0 \ \text{ for } \ u > 0, \tag{4.40}$$

and typically one takes $g(u) = u^n$ for some $n \geq 1$. See also Section 7.6.5 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 bacterial colonies, $u$ reprents the density of cells (and the colony is growing) and $v$ the nutrient consummed by the cells. See [26].

When $d_u = d_v$, a particular solution of system (4.39) consists in choosing $v = a - u$ ($a > 0$ a given positive number). Then it reduces to the Fisher/KPP equation (with temperature ignition in the case at hand) and thus it admits traveling waves. To avoid the parameter $a$, one can fix it equal to 1 and the traveling problem now reads

$$\begin{cases} -cu' - d_u u'' = g(u)v, \qquad u(-\infty) = 1, \quad u(+\infty) = 0, \\ \\ -cv - d_v v'' = -g(u)v, \qquad v(-\infty) = 0, \quad u(+\infty) = 1. \end{cases} \tag{4.41}$$

Translational invariance can be normalized by, say $u(0) = 1/2$.

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 [8] in the case of ignition temperature,

• Existence with $c$ large enough, and uniqueness, can be found in [36] in the case without ingnition temperature and $Le \leq 1$. A counterexample to uniquenes for $Le \geq 1$ is given in [11].

• The case $Le = 0$ is also useful for many applications and is treated in [35] and more recent analysis can be found in [2].

## 4.10 Two competing species

An example arising in ecology comes from two species in competition for the resources. The model considers two population densities $u_1$ and $u_2$ and reads (after normalization)

$$
\begin{cases} \frac{\partial}{\partial t}u_1 - d_1\Delta u_1 = r_1 u_1(1-u_1-\alpha_2 u_2), \\ \\ \frac{\partial}{\partial t}u_2 - d_2\Delta u_2 = r_2 u_2(1-\alpha_1 u_1-u_2). \end{cases} \tag{4.42}
$$

Notice 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 for instance that the species 1 is more motile than the species 2 that is $d_1 > d_2$. Depending on the predation coefficients $\alpha_1$, $\alpha_2$, and the specific growth rates $r_1$, $r_2$, is this an advantage? Does species 1 invade species 2 or the other way?

It can be noticed that there are several steady states

• the unpopulated steady state $(0,0)$ is always unstable,

• the one-species (monoculture) steady states are $(0,1)$ (esp. $(1,0)$). 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 above question is now to know which states can be connected by a traveling wave, 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 wants to connect the two stable states $(1,0)$ and $(0,1)$

$$
\begin{cases} -cv_1' - d_1 v_1'' = v_1(1-v_1-\alpha_2 v_2), \\ -cv_2' - d_2 v_2'' = v_2(1-\alpha_1 v_1 - v_2). \\ v_1(-\infty) = 1, \quad v_2(-\infty) = 0, \qquad v_1(+\infty) = 0, \quad v_2(+\infty) = 1. \end{cases}
$$

See [34], [4]. See also Section 7.7.1 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 $\lambda$, $\mu$, $\nu$

$$\frac{d}{dt}E(t) = -\big(\lambda + \mu u_1(t) + \nu u_2(t)\big)^2.$$

4. Derive from this equality the long time behaviour of the system.
*Solution.* We only solve the stability questions. The linearized matrix around $(U_1, U_2)$ is given by

$$L = \begin{pmatrix} -r_1U_1 & -\alpha_2 r_1 U_1 \\ \\ -\alpha_1 r_2 U_2 & -r_2 U_2 \end{pmatrix}$$

and $tr(L) = -(r_1U_1 + r_2U_2) < 0$, $det(L) = r_1r_2U_1U_2(1 - \alpha_1\alpha_2)$. Therefore
1. For $\alpha_1\alpha_2 < 1$, $det(L) > 0$ and the two eigenvalues have 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)

$$\begin{cases} \frac{\partial}{\partial t}u - d_u\Delta u &= r_1u(1 - 2av^2 - u), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \frac{\partial}{\partial t}v - d_v\Delta v &= r_2v(1 - 2bu^2 - v). \end{cases}$$

This system admits (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

$$r_1u(1 - 2av^2 - u)\frac{du}{dx} + r_2v(1 - 2bu^2 - v)\frac{\gamma\, dv}{dx} = \frac{d}{dx}P(u, v)$$

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 $x \in \mathbb{R}$,

$$\begin{cases} -cu' - d_uu'' &= r_1u(1 - 2av^2 - u), \qquad u(-\infty) = 1, \quad v(-\infty) = 0, \\ -cv' - d_vv'' &= r_2v(1 - 2bu^2 - v), \qquad u(\infty) = 0, \quad v(-\infty) = 1. \end{cases}$$

2. $\gamma = \frac{r_1 a}{r_2 b}$. $P(u, v) = r_1u - r_1au^2v^2 - r_1\frac{u^2}{2} + \gamma r_2 v - \gamma\frac{r_2}{2}v^2$.

3. We compute following section 4.1

$$\begin{aligned}-c\int[(u')^2+(v')^2]+0 &= \int u'[r_1u(1-2av^2-u)]+v'[r_2v(1-2bu^2-v)] = \\ &= \int \tfrac{dP}{dx}+P(0,1)-P(1,0)=\tfrac{r_1}{2}(\tfrac{a}{b}-1).\end{aligned}$$

So that $c$ has the sign of $b-a$.
4. This systems represents two species competing for space with carrying capacity normalized to 1. Independently of the reproduction rate, the species that uses more 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 to 15.000 years ago, recolonization of continents by trees and plants occured. Record 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 (Skellam, 1951) is the long distance dispersal effect by other species (birds, humans could bring seeds far away from the trees). A mathematical framework to quantify these effects can be found in Kot *et al*[8] and uses the formalism of section 4.10.

Another explanation are diffusion and growth from cryptic populations. Fossils records indeed indicate that small refugia existed[9]. Mathematical analysis can be found in Roques[10].

[8] Kot, M., Lewis, M. A. and Van der Driessche, Dispersal data and the spread of invading organisms. Ecology 77(7), 2027–2041 (1996).

[9] Benett K. D. and Provan J. What do we mean by refugia? Quaternary Science Reviews 27 (2008) 2449–2455.

[10] Roques L., Hamel F., Fayard J., Fady B. and Klein E. K. Recolonisation by diffusion can generate increasing rates of spread. Theoretical Population Biology, Vol 77 (2010) 205–212.

# Chapter 5

# Spikes and Pulses

## 5.1 Spike solutions

One of the typical behaviour of solutions to elliptic equations or systems are *spikes*. These are solutions that vanish at plus and minus infinity while traveling waves take different values at each end. We give several examples from different areas of biology.

### 5.1.1 A model for chemotaxis

We refer to [44] for more explanations on the subject of chemotaxis. Here we consider a density $u(x)$ of bacteria attracted by a chemoattractant which concentration is denoted by $v(x)$. The variant of the Keller-Segel model we use here takes into account the nonlinear diffusion of cells introducing an exponent $p$. In the modeling literature it is aimed at representing saturation effects in high density regions (volume filling, quorum sensing, signal limiting). It can also be derived from refined models at the mesoscopic (kinetic) or even microscopic (individual centered) scales. And we also consider one 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**. *1st step (Reduction to a single equation)* Solution $u$ can be obtained explicitely interms 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 on $v$ 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 behaviour 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 $v_x(0) = 0$, and this defines the unique value $v_0$ because of the assumption on $p$. 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 decide of the square root in equation (5.3) and we find

$$\begin{cases} v_x(x) = -\sqrt{\alpha v(x)^2 - g\big(v(x)\big)}, & v(0) = v_0, \quad x > 0, \\ v_x(x) = \phantom{-}\sqrt{\alpha v(x)^2 - g\big(v(x)\big)}, & v(0) = v_0, \quad x < 0. \end{cases}$$

This defines a unique function $v(x)$ which decreases to 0 as $|x| \to \infty$. $\square$

One can prove that the evolution equation asociated with (5.1) has the following behaviour. 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 Chapter 6) in finite time and concentrates as a Dirac mass. See [13].

**Exercise**. What does it happen for $p = 1$ 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

$$\begin{cases} -(u^{1+p})_{xx} + \big(u^q v_x\big)_x = 0, \qquad x \in \mathbb{R}, \\ -v_{xx} + \alpha v = u^r. \end{cases}$$

For which range of positive parameters $p$, $q$, $r$ are there spike solutions.

### 5.1.2 A non-local model from adaptive evolution

In order to motivate spikes, we may also take an example from the theory of adaptive evolution. A population is structured by a physiological parameter: it could be the size of an organ of the individuals, proportion of resource used for division, or any relevant parameter useful to describe the adaptation of the individuals i.e. their ability to use the nutrient for reproduction. We denote by $u(t, x)$ the density of individuals with trait $x \in \mathbb{R}$ (to make it as simple as possible), and we write the dynamics of the population density as, for instance to take the easiest model,

$$\begin{cases} \frac{\partial}{\partial t} v(t, x) - \Delta v = v\big(b(x) - \varrho(t)\big), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \varrho(t) = \int_{\mathbb{R}} v(t, x) dx, \\ v(t = 0, x) = v^0(x) \geq 0. \end{cases} \tag{5.4}$$

The term $\Delta v$ 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 of the trait $x$. Finally, $-\varrho$ models the death term, as in the Fisher/KPP equation, with the main difference that he 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

$$\begin{cases} -u''(x) = u(x)\ \big(b(x) - \overline{\varrho}\big), \qquad x \in \mathbb{R}, \\ \overline{\varrho} = \int_{\mathbb{R}} u(x) dx, \qquad u(x) > 0, \\ u(\pm\infty) = 0. \end{cases} \tag{5.5}$$

Notice that the problem (5.5) is simply an eigenvalue problem and is relevant from the Krein-Rutman theory (Perron-Froebenius theory in infinite dimension). The solution exists under quite general assumptions on $b$. We give in Figure 5.1 two examples of solutions for $b(x) = 20. * e^{-(x-.25)/.01}$ and $b(x) = 24 * e^{-(x-.25)/.01} + 20 * e^{-(x-.7)/.03}$.

We give a simple example with an explicit solution that explains the existence of a pulse solution

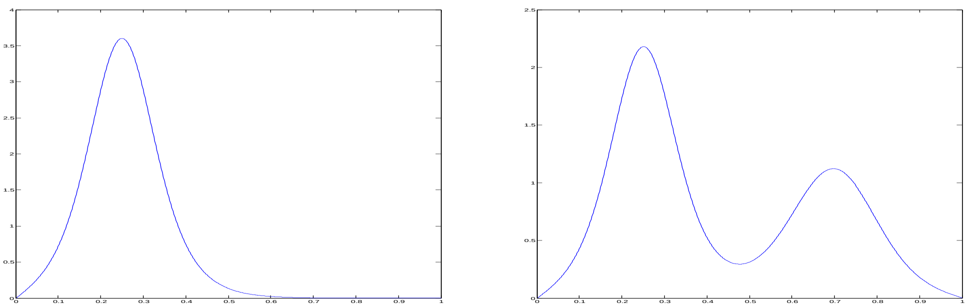

Figure 5.1: ONE AND TWO SPIKES SOLUTIONS OF EQUATION (5.5) FOR TWO DIFFERENT DATA $b(x)$.

**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 to (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 to (5.4) converges as $t \to \infty$ to the steady state solution to (5.5).*

**Proof of Theorem 5.2**. We first consider a solution, forgetting the condition $\overline{\varrho} = \int u$ and find an intrinsic condition on $\overline{\varrho}$. For $x \le -a$ the equation is $-u''(x) = u(x)(b_- - \overline{\varrho})$ and the conditions $u > 0$ and $u(-\infty) = 0$ impose $\overline{\varrho} > b_-$ and gives 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 need that $\overline{\varrho} < b_+$ and

$$u(x) = \mu_1 cos(\lambda_o x) + \mu_2 sin(\lambda_o x), \qquad -a \le x \le a, \qquad \lambda_o = \sqrt{b_+ - \overline{\varrho}}.$$

Also the sign condition $u(x) > 0$ imposes $\mu_1 > 0$ (at $x = 0$) and $\lambda_o a < \pi/2$ (otherwise take $\lambda_o x_o = \pm\pi/2$).

Now, we have to check the continuity of $u$ and $u'$ at the points $\pm a$. This gives the conditions

$$\begin{cases} \mu_- e^{-\lambda_- a} = \mu_1 \cos(\lambda_o a) - \mu_2 \sin(\lambda_o a), \\ \mu_+ e^{-\lambda_- a} = \mu_1 \cos(\lambda_o a) + \mu_2 \sin(\lambda_o a), \end{cases}$$

$$\begin{cases} \mu_- \lambda_- e^{-\lambda_- a} = \mu_1 \lambda_o \sin(\lambda_o a) + \mu_2 \lambda_o \cos(\lambda_o a), \\ \mu_+ \lambda_- e^{-\lambda_- a} = \mu_1 \lambda_o \sin(\lambda_o a) - \mu_2 \lambda_o \cos(\lambda_o a). \end{cases}$$

From these equalities we deduce first that the quantity $\mu = \frac{1}{2}(\mu_- + \mu_+)$ satisfies

$$\begin{cases} \mu e^{-\lambda_- a} = \mu_1 \cos(\lambda_o a), \\ \mu \lambda_- e^{-\lambda_- a} = \mu_1 \lambda_o \sin(\lambda_o a), \end{cases}$$

therefore $\lambda_- = \lambda_o \tan(\lambda_o a)$, in other words the parameter $\overline{\varrho}$ should satisfy

$$b_- \leq \overline{\varrho} \leq b_+, \qquad a\sqrt{b_+ - \overline{\varrho}} < \pi/2, \qquad \sqrt{\overline{\varrho} - b_-} = \sqrt{b_+ - \overline{\varrho}}\ \tan(a\sqrt{b_+ - \overline{\varrho}}).$$

By monotonicity we obtain that there is a unique $\overline{\varrho}$ satisfying these conditions, and that being given $\mu$, $\mu_1$ is proportional to $\mu$.

Next, we go back to the four conditions and now find

$$\begin{cases} \frac{\mu_+ - \mu_-}{2} e^{-\lambda_- a} = \mu_2 \sin(\lambda_o a), \\ \frac{\mu_+ - \mu_-}{2} \lambda_- e^{-\lambda_- a} = -\mu_2 \lambda_o \cos(\lambda_o a), \end{cases}$$

and straightforward sign considerations show that $\mu_2 = 0$ and $\mu_- = \mu_+$.

Therefore we have the only free parameter $\mu$ left. It is needed to realize the mass condition $\overline{\varrho} = \int_{\mathbb{R}} u(x)dx$ and thus we have indeed a unique solution. $\square$

**Proof of Theorem 5.3**. Consider the solution $\widetilde{v}(t,x) \geq 0$ to the heat equation

$$\begin{cases} \frac{\partial}{\partial t} \widetilde{v}(t,x) - \Delta \widetilde{v} = \widetilde{v}\big(b(x) - \overline{\varrho}\big), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \widetilde{v}(t=0,x) = v^0(x) \end{cases} \tag{5.6}$$

This is a heat equation with 0 the first eigenvalue of the steady equation. We know from the maximum principle that $0 \leq \widetilde{v}(t,x) \leq C_0 u(x)$ (see the proof of Lemma). And from the general theory of dominant eigenvectors of positive operators (Perron-Froebenius),

$$v(t,x) \xrightarrow[t\to\infty]{} \lambda u(x),$$

for some $\lambda \in \mathbb{R}$.

On the other hand we can look for the solution to (5.4) under the form $v(t,x) = \mu(t)\widetilde{v}(t,x)$ with $\mu(t) \geq 0$. We have

$$\frac{\partial}{\partial t} v(t,x) - \Delta v - v\big(b(x) - \varrho(t)\big) = \dot{\mu}(t)\widetilde{v}(t,x) + \mu(t)\widetilde{v}(t,x)\big(\varrho(t) - \overline{\varrho}\big),$$

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 $\varrho(t) = \int_{\mathbb{R}} v(t,x)dx = \mu(t) \int_{\mathbb{R}} \widetilde{v}(t,x)dx = \mu(t)\lambda(t)$, with

$$\lambda(t) = \int_{\mathbb{R}} \widetilde{v}(t,x)dx \underset{t\to\infty}{\longrightarrow} \lambda.$$

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

$$\mu(t) \underset{t\to\infty}{\longrightarrow} \overline{\varrho}/\lambda.$$

This is exactly the announced result. $\square$

**Exercise**. Consider the model

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - \Delta u = u\big(\frac{b(x)}{1+\varrho(t)} - d(x)\varrho(t)\big), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \varrho(t) = \int_{\mathbb{R}} u(t,x)dx. \end{cases} \tag{5.7}$$

Assume that $b$, $d$ still take two different values (with same discontinuity points) and give a condition for existence of a spike solution.

## 5.2 Traveling pulses

We describe the mathematical mechanism for creating *pulses* which means spikes that are moving as a traveling wave. The upmost famous example, namely Hodgkin-Huxley system, describes acurately propagation of ionic signal along nerves. It is rather complex and we prefere here to retain only simplified models, which we hope, explains better the mechanism.

### 5.2.1 Fisher/KPP pulses

A method to create a pulse from the Fisher/KPP equation is to include a component $v(t,x)$ which allows to drive back the state $u = 1$ 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 impose that $u$ itself decreases to zero. With these considerations, we arrive to the system

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - \Delta u &= u[1-u-v] \\ \\ \frac{\partial}{\partial t}v(t,x) &= u, \end{cases} \tag{5.8}$$

The solutions at a given time are depicted in Figure 5.2. One can observe that $u$ is indeed a pulse but $v$ does not vanish at $x = -\infty$ by opposition with FitzHugh-Nagumo system.

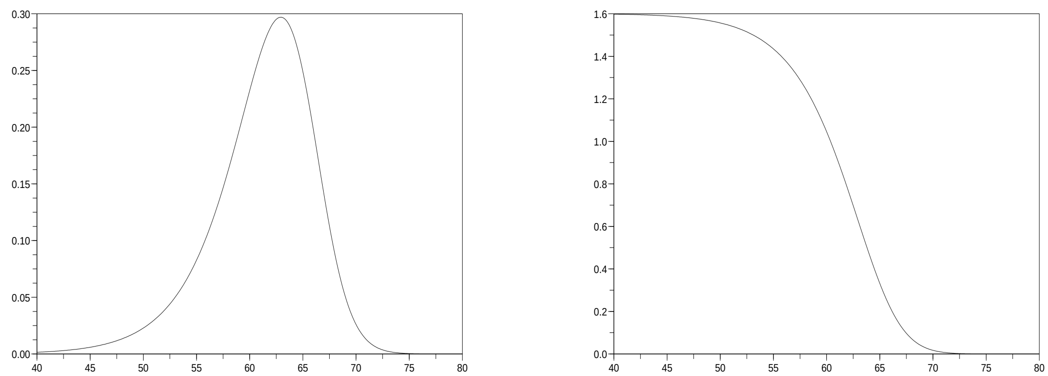


Figure 5.2: Fisher/KPP pulses, these are traveling wave solutions to the system (5.8). The solution is presented as a function of $x$, at a given time. The pulse propagates from left to right. Left: $u(t,x)$ exhibits a pulse shape, i.e., it vanishes at both endpoints. Right: $v(t,x)$ exhibits a traveling wave as in Fisher/KPP equation but not a pulse shape (by opposition with FitzHugh-Nagumo system).

### 5.2.2 FitzHugh-Nagumo system

Several parabolic models have been used in neurosciences with a huge impact for the propagation of nerve impulses. Hodgkin-Huxley system, the first model, gave amazing results with comparisons to experiments along the giant squid axon during the 1950's (see [41]). This model has initiated the theories of electrophysiology, cardiac, neural communication by electrical signaling or neural rhythms.

The FitzHugh-Nagumo system is nowadays the simpler model used to describe pulses 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 Figure 5.3 (Left) we depict a pulse traveling with parameters indicated in the figure caption. We choose here $\alpha < .5$ in order to propagate a traveling wave in the Allen-Cahn equation on $u$ (initially $v \equiv 0$). This switches on the equation on $v$, and with a certain delay it inhibits the pulse and $u$ goes back to the other stable value $u = 0$. For that we need the condition

$$u(1-u)(u-\alpha) < \frac{\gamma}{\beta}u \quad \text{for } \ 0 < u < 1.$$

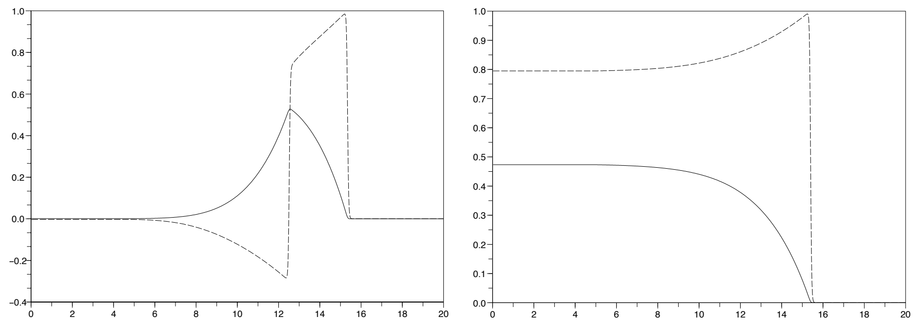

Figure 5.3: Solutions of the FitzHugh-Nagumo equation (5.9) with with $\varepsilon = 0.02$, $\alpha = 0.1$ and $\beta = .2$ and (Left) $\gamma = .25 * \beta$, (Right) $\gamma = .15 * \beta$. According to the explanation in the text, for $\gamma$ large we obtain a traveling pulse, for $\gamma$ small we obtain a traveling wave. Dashed line is $u$, continuous line is $v$ (amplified by a factor 4). See also Figure 5.4. The original Fitz-Hugh Nagumo system exhibits an undershoot of $u$ which is observed in neurons and is called hyperpolarization.

In the other case we can reach and equibrium $\beta v = \gamma u$ which transforms the bistable nonlinearity in a monostable.

The parameter $\varepsilon$ controls the stifness of the fronts, $\beta$ the width of the pulse and $\frac{\gamma}{\beta}$ the type of wave.

As one can see on Figure 5.3, the solution $u$ is negative. this is in accordance with electric 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 instance for cardiac electric waves) This is the reason why several variants exist.

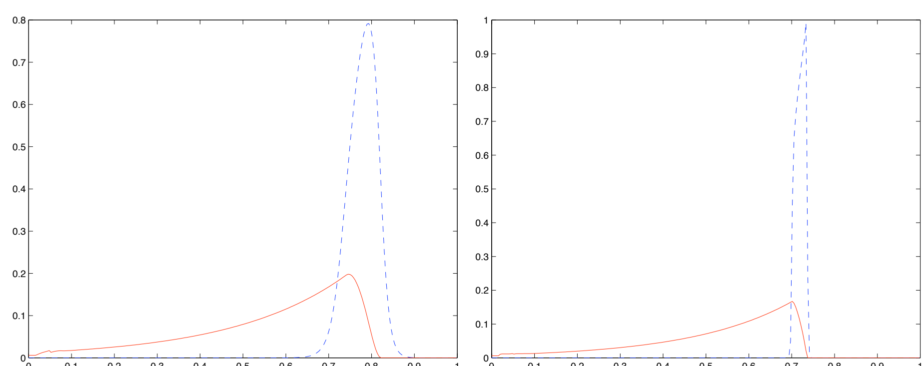

Figure 5.4: Solutions of the space structured FitzHugh-Nagumo system (5.10) with $\alpha = .2$ and $\varepsilon = 0.01$ (left), $\varepsilon = 0.001$ (right); we represent both $u(t, x)$ (dashed line) and $v(t, x)$ (continuous line) as a function of $x$, at a given time. The pulse propagates from left to right.

A possible way to garantee that $u$ remains nonnegative is to modify the FitzHugh-Nagumo system into

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - \varepsilon\Delta u &= \frac{1}{\varepsilon}u[(1-u)(u-\alpha)-v] \\ \\ \frac{\partial}{\partial t}v(t,x) &= v_\infty(u) - v, \end{cases} \tag{5.10}$$

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 McCulloch[1].

• For $v_\infty(u) = ku(u-1-a)$, the system is called Aliev-Panfilov[2].

Figure 5.4 shows a pulse for equation (5.10) with $\alpha = .2$, $v_\infty(u) = 3. * (u - .4)_+$ (here the numbers are adapted to $\alpha = .2$) which propagates from left to right. Two values of $\varepsilon$ are represented.

[1] J. M. Roger and A. D. McCulloch. A collocation-Galerkin finite element model of cardiac action potential propagation. IEEE Trans. biomed. Engr 41 (19914) 743–757.

[2] R. Aliev and A. Panfilov. A simple two-variable model of cardiac excitation. Chaos, solitons and fractals, 3(7) (1996) 293–301.

# Chapter 6

# Blow-up and extinction of solutions

We know from Chapter 2 that for 'small' nonlinearities, the solutions to parabolic systems relax to an elementary state. When the nonlinearity is too large, it is possible that solutions to 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 on simple ordinary differential equations. Blow-up means that the solution becomes larger and larger pointwise 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 *blows-up* in finite time, i.e., solutions tend 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 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 $t \to 0$.

The purpose of this Chapter is to study in which respect these phenomena can occur for not or parabolic equations.

We begin with the semilinear parabolic equation with Dirichlet boundary condition

$$\frac{\partial}{\partial t}u - \Delta u = u^2.$$

We present several methods for proving blow-up in finite time. The first two methods are on semi-linear parabolic equations, the third method is illustrated on 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 (it represents the total number of cells in a system where division 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

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = u^2, \qquad t \geq 0,\ x \in \Omega, \\ u(x) = 0, \qquad x \in \partial\Omega, \\ u(t=0,x) = u^0(x) \geq 0. \end{cases} \tag{6.2}$$

Here we treat the case when $\Omega$ 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 need 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 to (6.2)*, a function satisfying for some $T > 0$,

$$u \in L^2([0,T) \times \Omega), \qquad u \in C\big([0,T]; L^1(\Omega)\big). \tag{6.3}$$

The question is then to know if diffusion is able to win against the quadratic nonlinearity and (6.2) could have global solutions. The answer is given by the next theorems

**Theorem 6.1** *Assume that $\Omega$ is a bounded domain, $u^0 \geq 0$, $u^0$ is large enough (in a weighted $L^1$ space introduced below), then there is a time $T^*$ for which the solution to (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 $L^p$ noms, $2 \leq p \leq \infty$ because we are in a bounded domain. It is also possible to prove that the blow-up time is the same for all these norms [47].

**Proof of Theorem 6.1**. We are going to obtain a contradiction on the hypothesis that a function $u \in L^2([0,T) \times \Omega)$ can be a solution to (6.2) when $T$ overpasses an explicit value we compute below.

Because we are working in a bounded domain, the operator $-\Delta$ has a smallest eigenvalue associated with a positive eigenfunction (see Section 2.5)

$$\begin{cases} -\Delta w_1 = \lambda_1 w_1, & w_1 > 0 \quad \text{in } \in \Omega \\ w_1(x) = 0,\ x \in \partial\Omega, & \int_\Omega (w_1)^2 = 1. \end{cases} \tag{6.4}$$

For a solution, we can multiply equation (6.2) by $w_1$ and integrate by parts. We arrive at

$$\begin{aligned} \frac{d}{dt} \int_\Omega u(t,x)\ w_1(x)\ dx &= \int_\Omega \Delta u(t,x)\ w_1(x)\ dx + \int_\Omega u(t,x)^2\ w_1(x)\ dx \\ &= \int_\Omega u(t,x)\ \Delta w_1(x)\ dx + \int_\Omega u(t,x)^2\ w_1(x)\ dx \\ &= -\lambda_1 \int_\Omega u(t,x)\ w_1(x)\ dx + \int_\Omega u(t,x)^2\ w_1(x)\ dx \\ &\geq -\lambda_1 \int_\Omega u(t,x)\ w_1(x)\ dx + \left(\int_\Omega u(t,x)\ w_1(x)\ dx\right)^2 \left(\int_\Omega w_1(x)\ dx\right)^{-1} \end{aligned}$$

(after using the Cauchy-Schwarz inequality). We set $z(t) = e^{\lambda_1 t} \int_\Omega u(t,x)\ w_1(x)$ and, with $a = \left(\int_\Omega w_1(x)\ dx\right)^{-1}$, the above inequality reads

$$\frac{d}{dt} z(t) \geq a e^{-\lambda_1 t}\ z(t)^2,$$

and we obtain:

$$\frac{d}{dt} \frac{1}{z(t)} \leq -a e^{-\lambda_1 t},$$

$$\frac{1}{z(t)} \leq \frac{1}{z^0} - a \frac{1 - e^{-\lambda_1 t}}{\lambda_1}.$$

Assume now the size condition

$$z^0 > \frac{\lambda_1}{a}. \tag{6.5}$$

The above inequality contradicts that $z(t) > 0$ for $e^{-\lambda_1 t} \leq 1 - \frac{\lambda_1}{a z^0}$. 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 see it. For $d \leq 5$ it follows from a general elliptic equation

**Theorem 6.2** *There is a steady state solution $\bar{u} > 0$ in $\Omega$ 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 [17] 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 $\widetilde{w} = \mu w_1$.This is a supersolution to (6.2) because

$$\frac{\partial}{\partial t}\widetilde{w} - \Delta \widetilde{w} = \lambda_1 \widetilde{w} \geq \widetilde{w}^2.$$

One concludes that any solution to (6.2) with $u^0 \leq \widetilde{w}$ satisfies $u(t) \leq \widetilde{w}$ for all times $t$ where the solution exists (and this is enough to prove that the solution is global). Therefore we have the

**Lemma 6.3** *Under the smallness condition $u^0 \leq \min_\Omega \frac{\lambda_1}{w_1(x)} w_1$, there is a global solution to (6.2) and $u(t) \leq \widetilde{w}$, $\forall t \geq 0$.*

**Proof**. We substract a solution $u$ to $\widetilde{w}$ and find

$$\frac{\partial}{\partial t}[u - \widetilde{w}] - \Delta[u - \widetilde{w}] \leq u^2 - \widetilde{w}^2 = [u - \widetilde{w}][u + \widetilde{w}],$$

with $u - \widetilde{w}(t = 0) \leq 0$. From the comparison principle, we conclude that $u - \widetilde{w}(t) \leq 0$ 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

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = f(u), \qquad t \geq 0, \ x \in \Omega, \\ u(x) = 0, \qquad x \in \partial\Omega, \\ u(t = 0, x) = u^0(x) > 0 \quad \text{ large enough}, \end{cases} \tag{6.6}$$

and $f(u) \geq c u^\alpha$ with $\alpha > 1$.

**Exercise**. (Neumann boundary condition) A solution on $[0, T)$ to the equation

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = u^2, \qquad t \geq 0, \ x \in \Omega, \\ \frac{\partial}{\partial \nu}u(x) = 0, \ x \in \partial\Omega, \\ u(t = 0, x) = u^0(x) > 0. \end{cases} \tag{6.7}$$

is a distributional solution such that $u \in L^2([0, T) \times \Omega)$.
1. Prove that there is no such solution after some time $T^*$ and no size condition is needed 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 non-zero solution to

$$-\Delta v = v^2, \qquad v(\pm 1) = 0.$$

*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 for semilinear parabolic equations, we consider another method leading to a different size condition. It uses better the intrinsic properties of the equation and does not use the sign condition.

We consider a more general case with $p > 1$

$$\begin{cases} \frac{\partial}{\partial t}u - \Delta u = |u|^{p-1}u, \qquad t \geq 0,\ x \in \Omega, \\ u(x) = 0,\ x \in \partial\Omega, \\ u(t=0,x) = u^0(x) \neq 0. \end{cases} \tag{6.8}$$

Before we state our result, it is useful to recall the energy principle underlying this equation. We define the energy

$$E(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 - \frac{1}{p+1}\int_\Omega |u|^{p+1}.$$

Notice that it has a mecanical 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

$$\begin{aligned} \tfrac{d}{dt}E\big(u(t)\big) &= \int_\Omega \big[\nabla u.\nabla \tfrac{\partial u}{\partial t} - |u|^{p-1}u\tfrac{\partial u}{\partial t}\big] \\ &= -\int_\Omega \tfrac{\partial u}{\partial t}\big[\Delta u + |u|^{p-1}u\big] \\ &= -\int_\Omega \big[\Delta u + |u|^{p-1}u\big]^2 \leq 0. \end{aligned}$$

Consequently, we have

$$E(t) \leq E^0 := E(u^0). \tag{6.9}$$

This explains the central role of the energy in the

**Theorem 6.4** *For $u^0 \in H_0^1(\Omega)$ satisfying $E(u^0) \leq 0$, there are no global solution to* (6.8) *with bounded energy.*

**Proof**. We define $\alpha = \frac{1}{2} - \frac{1}{p+1} > 0$. The energy decay shows that

$$\begin{aligned}\frac{1}{4}\frac{d}{dt}\int_\Omega u^2 &= -\int_\Omega |\nabla u|^2 - |u|^{p+1} \\ &= -E(u) + \alpha \int_\Omega |u|^{p+1} \\ &\geq -E(u^0) + \alpha|\Omega|^{(1-p)/2}\left(\int_\Omega u^2\right)^{(p+1)/2}.\end{aligned}$$

The last inequality uses Jensen's inequality for the probability measure $dx/|\Omega|$

$$\left(\int_\Omega u^2 \frac{dx}{|\Omega|}\right)^{(p+1)/2} \leq \int_\Omega u^{p+1}\frac{dx}{|\Omega|}.$$

This proves blow-up for $E(u^0) \leq 0$ because the positive function $z(t) := \int_\Omega u^2$ satisfies

$$\frac{dz(t)}{dt} \geq \beta\,(z(t))^{(p+1)/2}, \qquad \beta := \alpha|\Omega|^{(1-p)/2} > 0,$$

and thus it blows-up in finite time, as shown in the introduction. □

**Exercise**. Find functions $u^0 \in H_0^1(\Omega)$ that satisfy the condition $E(u^0) \leq 0$.
*Hint.* Use that the two terms in the energy have different scales in $u$.

**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 [47].

## 6.3 Keller-Segel system; the moment method

We come back to the Keller-Segel model used to describe chemotaxis as mentioned in Section 8.8. We recall that it consists in a system which describes the evolution of the density of cells (bacteria, amoebia,...) $n(t,x)$, $t \geq 0$, $x \in \mathbb{R}^d$ and the concentration $c(t,x)$ of the chemical attracting substance emited by the cells themselves,

$$\begin{cases} \frac{\partial}{\partial t}n - \Delta n + \operatorname{div}(n\chi\nabla c) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ -\Delta c + \tau\, c = n, \\ n(t=0) = n^0 \in L^\infty \cap L^1_+(\mathbb{R}^d). \end{cases} \tag{6.10}$$

The first equation just expresses the random (brownian) diffusion of the cells with a bias directed by the chemoattractant concentration with a sensitivity $\chi$ (the case $\chi = 0$ means the cells do not react). The chemoattractant $c$ is directly emitted by the cell, diffused on the substrat and degraded with a coreffficient $\tau$ scales in a such a way that $\tau^{-1/2}$ represents its activation length.

The notation $L^1_+$ means nonnegative integrable functions, and the parabolic equation on $n$ gives nonnegative solutions (as expected for the cell density, see Chapter 8)

$$n(t,x) \geq 0, \qquad c(t,x) \geq 0. \tag{6.11}$$

Another property we will 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 to (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 to (6.10) satisfying the a priori estimates*

$$\int_{\mathbb{R}^2} n[|\ln(n(t))| + |x|^2]\, dx \leq C(t),$$

$$\|n(t)\|_{L^p(\mathbb{R}^2)} \leq C(p,t,n^0) \qquad \textit{for} \ \ \|n^0\|_{L^p(\mathbb{R}^2)} < \infty, \quad 1 < p < \infty.$$

Here we only explain the argument for blow-up and refer to [45, 10] for the other results. In fact the subject is very rich and many other mathematical questions have been treated.

**Proof**. Formally the blow-up proof is very simple, and the difficulty here is to prove that the solution becomes a singular measure. We follow Nagai's argument, first assuming enough decay in $x$ at infinity, afterward we state a more precise result. It 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),

$$\begin{aligned} \frac{d}{dt} m_2(t) &= \int_{\mathbb{R}^2} \frac{|x|^2}{2} [\Delta n - \mathrm{div}(n\chi \nabla c)]dx \\ &= \int_{\mathbb{R}^2} [2n + \chi n x \cdot \nabla c]dx \\ &= 2m^0 - \chi\lambda_2 \int_{\mathbb{R}^2\times\mathbb{R}^2} n(t,x)n(t,y) \frac{x\cdot(x-y)}{|x-y|^2} \\ &= 2m^0 - \frac{\chi\lambda_2}{2} \int_{\mathbb{R}^2\times\mathbb{R}^2} n(t,x)n(t,y) \frac{(x-y)\cdot(x-y)}{|x-y|^2} \end{aligned}$$

(this last equality just 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. Therefore the solution cannot be smooth until that time. $\square$

## 6.4 Non-extinction

We consider now a nonlinearity with the other 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 [31], 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 to* (6.15) *satisfies*

$$\lim_{t\to\infty} M(t) > 0.$$

There is a nice biological interpretation in [31] related to 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 lifespan 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 are negatively buoyant and fall 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 such high rates, rapid dispersion at the ocean surface is needed for encounter and certainly chemotactic attraction too. The model supposes that sperm and eggs have the same density (but this assumption can be release in a system of two parabolic equations, arriving at the same conclusion). 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 chemotactism, not all the eggs are fertilized. In [31] it is proved that chemoattraction increases this rate but additional flow mixing does not.

**Proof**. First of all, we can estimate for all $t > \tau > 0$ thanks to (3.21) with initial time $\tau$,

$$\int_{\mathbb{R}^d} u^p(t,x)dx \leq C(d,p)\ M(\tau)^p\ t^{-(p-1)d/2}.$$

Therefore

$$M(T) = M(\tau) - \int_\tau^T \int_{\mathbb{R}^d} u^p(t,x)dxdt \geq M(\tau) - C(d,p)M(\tau)^p \int_\tau^T t^{-(p-1)d/2}dt.$$

Because our assumption on $p$ is equivalent to $\delta = (p-1)d/2 - 1 > 0$, we can also write this inequality as

$$M(T) \geq M(\tau) - C_1(d,p)M(\tau)^p \frac{1}{\tau^\delta}.$$

Next, notice that the system cannot get extinct in finite time because $0 < u(t,x) < \|u^0\|_\infty$ and thus

$$\frac{d}{dt}M(t) = -\int_{\mathbb{R}^d} u^p(t,x)dx \geq -\|u^0\|_\infty^{p-1} M(t),$$

which implies that $M(t) \geq M(0)e^{-t\|u^0\|_\infty^{p-1}}$.

Hence, we can consider the first time $\tau \geq 2$ such that $M(\tau)^{p-1} \leq 1/C_1(d,p)$ (if such a time does not exist, the result is proved). We have for all $T \geq \tau$

$$M(T) \geq M(\tau)\big(1 - \frac{1}{\tau^\delta}\big) \geq M(\tau)\big(1 - \frac{1}{2^\delta}\big).$$

This proves the result. $\square$

**Exercise**. From the above argument derive an explicit bound on 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 gametes

$$\begin{cases} \frac{\partial}{\partial t} e - d_e \Delta e = -(eg)^{p/2}, & t \geq 0, \; x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} g - d_g \Delta g = -(eg)^{p/2}, & \\ e(t=0,x) = e^0(x) > 0. & g(t=0,x) = g^0(x) > 0 \end{cases}$$

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 [31] again.

# Chapter 7

# Linear instability, Turing instability and pattern formation

In his seminal paper[1] 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 morphegnesis'. He introduces several concepts as 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 is published in 1972 with the celebrated system of Gierer and Meinhardt [24] (see also section 7.6.8).

It is only 20 years later that the first experimental evidence of a chemical reaction exhibiting spatial patterns explained by these principles was obtained. It is named the CIMA reaction after the name of the reactants used by P. De Kepper et al[2]. See also section 7.6.2.

In 1995, S. Kondo and R. Asai[3] proposed to explain the patterns arising during the development of animals using a growing domain, thus opening a larger class of possible patterns. Spots which are usual steady states for Turing systems on a fixed domain, can more easily leave place to bands on a growing domain.

Meanwhile, several nonlinear parabolic systems exhibiting Turing Patterns have been studied. Some have been aimed at modelling particular examples of morphogenesis as the models

[1] Turing A. M. The chemical basis of morphogenesis, Phil. Trans. Roy. Soc. London, B237, 37–7 (1952).

[2] P. De Kepper, V. Castets, E. Dulos and J. Boissonade. Turing-type chemical patterns in the chlorite-iodide-malonic acid reaction, Physica D 49 (1991), 161–169.
V. Castets, E. Dulos, J. Boissonade and P. De Kepper. Experimental evidence of a sustained standing Turing-type nonequilibrium chemical pattern. Phys. Rev. Letters 64(24) 2953–2956 (1990).

[3] Kondo, S and Asai R. A reaction-diffusion wave on the skin of the marine anglefish *Pomocanthus*, Nature (1995)

developed in [37, 38]. Some have been derived as the simplest possible models exhibiting Turing instability conditions.Nowadays, the biological interest for morphognesis have evolved towards molecular cascades, pathways and networks. Biologists doubt that, within cells or tissues, diffusion is adequate to describe molecular spreading. It remains that Turing's mechanism stays both the simplest explanation for pattern formation, and one of the most counter-intuitive results in PDEs.

This chapter presents this 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 is the nonlocal Fisher/KPP equation, some more standard parabolic systems are also presented.

Figure 7.1: Examples of patterns in nature that have motivated the study of systems exhibiting Turing patterns.

## 7.1 Turing instability in linear reaction-diffusion systems

An amazingly counter-intuitive observation is the instability mechanism proposed by A. Turing [51]. Consider a linear $2 \times 2$ O.D.E. systems

$$\begin{cases} \frac{du}{dt} = au + bv, \\ \frac{dv}{dt} = cu + dv, \end{cases} \tag{7.1}$$

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 $\Omega$ 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 Neuman or Dirichlet boundary conditions. In both cases the state $(u, v) = (0, 0)$ is still a steady solution, to (7.4) now.

In principle adding diffusion in the differential system (7.1) should help for stability. But surprisingly we have the

**Theorem 7.1** *Consider the system (7.4) where we fix the domain $\Omega$, the matrix $A$ and $\sigma_v > 0$. We assume (7.2) with $a > 0$, $d < 0$. Then, for $\sigma_u$ small enough, 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 $\sigma$'s scale as square of length. The result can be extended as the

**Turing instability alternative.**

- Turing instability $\Longleftrightarrow$ short range activator, long range inhibitor.
- Traveling waves $\Longleftrightarrow$ long range activator, short range inhibitor.

There is no general proof of such a result which can only be applied to nonlinear systems. But it is a general observation that can be verified case by case. Also, we mean 'stable traveling waves', because traveling waves can also exist in the former case but they are unstable in the sense that the dynamics creates Turing patterns.

**Proof of theorem 7.1.** We consider the Laplace operator, with Dirichlet or Neuman conditions 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 $\lambda_k$,

$$-\Delta w_k = \lambda_k w_k.$$

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 enough, 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 vansihes

$$0 = \det \begin{pmatrix} \lambda + \sigma_u \lambda_k - a & -\,b \\ & \\ -c & \lambda + \sigma_v \lambda_k - d \end{pmatrix}$$

Hence, there is a solution with exponential growth for those eigenvalues $\lambda_k$ 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

$$(\lambda_k)^2 - \lambda_k(\frac{d}{\sigma_v} + \frac{a}{\sigma_u}) + \frac{\mathcal{D}}{\sigma_u\sigma_v} < 0. \tag{7.8}$$

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 large enough with $\frac{\mathcal{D}}{\sigma_u\sigma_v}$ small enough. It is hardly possible to give an accurate general characterization in terms $\sigma_u$ and $\sigma_v$ for $(a, b, c, d)$ fixed because we do not know the repartition of the eigenvalues a priori.

To go further, we set

$$\theta = \frac{\sigma_u}{\sigma_v},$$

and we write explicitely the roots of the above polynomial and we need 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 $\theta$ 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 $\sigma_u$ small, $\sigma_v$ of order 1, the interval $[\Lambda_-, \Lambda_+]$ becomes very large, hence we know that some eigenvalues $\lambda_k$ will belong to this interval.

Notice however that, because $\lim_{k\to\infty} \lambda_k = +\infty$, there are only a finite number of unstable modes $\lambda_k$. $\square$

In principle one will observe the mode $w_{k^0}$ corresponding to the largest possible $\lambda$ in (7.7) among the $\lambda_k$ satisfying the condition (7.9). This does not correspond necessarily to the largest value of $\lambda_k$ satisfying the inequality (7.8).

**Exercise**. Compute the first two terms in the expansion of $\lambda$ 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 $Re(\lambda) > 0$.

Figure 7.2: Examples of animals with spots and stripes. Left: Discus (http://animal-world.com/encyclo/fresh/cichlid/discus.php). Right: Ocelot (http://notrenature.cowblog.fr/426-ocelot-3055620.html).

Figure 7.3: Another animal with spots and stripes.

## 7.2 Spots on the body and stripes on the tail

Turing instability provides us with a possible explanation of why so many animals (especially fishes) have spots on the body and stripes on the tail, see Figures 7.2–7.4. In short words, in a long and narrow domain (a tail) typical eigenfunctions are 'bands' and with a better shaped domain (a mathematical square body), the eigenfunctions are 'spots' or 'chessboards'. A much better and more detailed discussion with precise biological cases demonstrated, and also the original papers where this idea stems from, can be found in [41] Vol. II Chapter 3.

To explain this, we consider Neuman boundary condition and use our computations of eigenvalues in Section 2.5.2. In one dimension, on a domain $[0, L]$, the eigenvalues and eigenfunctions are

$$\lambda_k = \left(\frac{\pi k}{L}\right)^2, \qquad w_k(x) = \cos\left(\frac{\pi k x}{L}\right), \qquad k \in \mathbb{N}.$$

Figure 7.4: MANY SPECIES OF SNAKES HAVE STRIPES.

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 $\lambda_{kl}$ 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 repartition of sums of squared integers generically imposes that the $\lambda_{kl} \in [\Lambda_-, \Lambda_+]$ will be for $l \approx k$ .

To conclude this section, we point out that growing domains during the development also influences very strongly the pattern formation. Again, we refer to [41] for a detailed analysis of the Turing patterns, and their interpretation in development biology.

## 7.3 The simplest nonlinear example: the nonlocal Fisher/KPP equation

Figure 7.5: AN EXAMPLE OF LABYRINTHIC PATTERNS IN TIGER BUSH IN NIGER, SEE [33].

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 and the convolution kernel $K$ is 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 it takes into account that competition for resources can be of long range (the size of the support of $K$) and not just local.

It has been proposed in ecology as an improvment of the Fisher equation that takes into account long range competition for resources [12, 27]. In semi-arid regions the roots of the trees, in competition for water, can cover up 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' lanscape [33], see Figure 7.5.

It has also been proposed as a simple model of adaptive evolution to take account for higher competition between closer trait [22]; $x$ represents a physiological trait, the Laplace term represents mutations and the right hand side growth and competition. The convolution kernel means that competition between individuals of closer phenotypical traits is higher than between more different traits (see also Section 5.1.2).

The convolution term has a drastic effect on solutions; it can induce that solutions exhibit a behavior quite different from those to 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 reads $f(0) = 0$, $f'(0) > 0$ 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 in between the unstable ones. This is the case of the nonlinearities arising in Fisher/KPP equation that we have encountered.

In the infinite dimensional framework at hand, we will see that under certain circumstances, the steady state $u \equiv 1$ can be unstable in the sense of the

**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) threre 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 behaviors because they remain bounded away from the two extreme steady states, cannot converge to the steady state $u^0$ and cannot oscillate rapidly. In other words, they should exhibit Turing patterns. See Figure 7.6 for a numerical solution to (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 it in section 7.1. On the full line, we may use the generalized eigenfunctions which are the Fourier modes. We define the Fourier transform as

$$\widehat{u}(\xi) = \int_{\mathbb{R}} u(x) e^{-ix\,\xi} dx.$$

**Theorem 7.4** *Assume the condition*

$$\exists \xi_0 \quad \text{such that } \widehat{K}(\xi_0) < 0, \tag{7.11}$$

*and $\nu/r$ small enough (depending on $\xi_0$ and $K(\xi_0)$), then 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 on numerical simulations, see Figure 7.6.

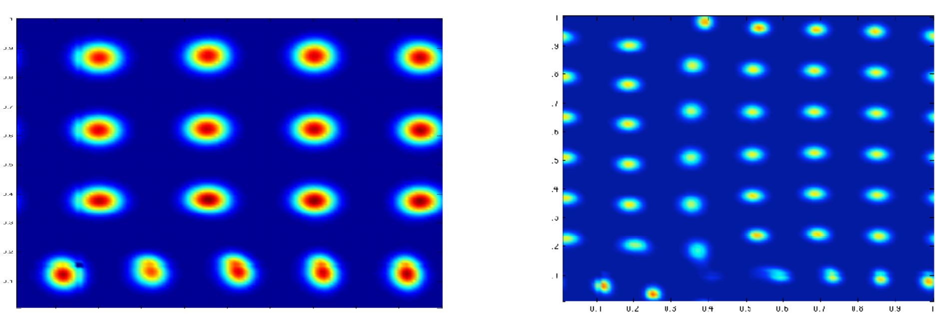

Figure 7.6: Steady state solutions of the nonlocal Fisher/KPP equation (7.10) in 2 dimensions with different diffusion coefficients.

The nonlocal Fisher equation gives also an example of the already mentioned alternative

**Turing instability alternative.**

- Turing instability $\iff$ $K(\cdot)$ is long range.
- Traveling waves $\iff$ $K(\cdot)$ is short range.

Inded the nonlocal 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 [7].

**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 setting $u = 1 + \widetilde{u}$ and keeping the first order temrs, we obtain

$$\frac{\partial}{\partial t}\widetilde{u} - \nu \frac{\partial^2}{\partial x^2}\widetilde{u} = -r\ K * \widetilde{u}.$$

And we look for solutions of the form $\widetilde{u}(t,x) = e^{\lambda t} v(x)$ with $\lambda > 0$. This means that we should find eigenfunctions associated with the positive eigenvalue $\lambda$ to

$$\lambda v - \nu \frac{\partial^2}{\partial x^2} v = -r\ K * v.$$

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

$$\lambda + \nu \xi_1^2 = -r\ \widehat{K}(\xi_1), \qquad \text{for some } \ \lambda > 0. \tag{7.12}$$

And it is indeed possible to such a $\lambda$ and a $\xi_1 = \xi_0$ under the conditions of the Theorem.
(iii) The possible unstable modes $\xi_0$ are obviously bounded because $\widehat{K}$ is bounded as the Fourier transform of a probability density ($|\widehat{K}| \leq 1$). $\square$

Notice however that the mode $\xi_1$ we will observe in pratice is that with the highest growth rate $\lambda$.

## 7.4 Connecting a Turing unstable state to a dynamically unstable state

We continue our analysis of traveling wave based on analytical solutions as we did it at the begining of Chapter **??** Here we consider the problem of connecting a Turing unstable state to a dynamically unstable state. The problem we solve is

$$-u''(x) - c'(x) = \begin{cases} 0 & \text{for } \ 0 \leq u < \theta, \\ (1 - K * u) & \text{for } \ \theta < u. \end{cases}, \qquad x \in \mathbb{R}, \tag{7.13}$$

$$u(-\infty) = 1, \qquad u(+\infty) = 0, \qquad u(0) = \theta.$$

## 7.5 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 my 'blow-up' by high frequency oscillations?

As an example of such an instable system, which is not Turing instable, we consider the phase transition model also used in Section 8.9,

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta A(u) = 0, \qquad x \in \Omega, \\ \\ \frac{\partial}{\partial \nu} u = 0 \qquad \text{on } \partial\Omega, \end{cases} \tag{7.14}$$

with

$$A(u) = u\,(3-u)^2. \tag{7.15}$$

Because $A'(u) = 3(3-u)(1-u)$, the equation (7.14) is backward-parabolic in the interval $u \in (1,3)$ because $A'(u) < 0$ there. We expect that linear instability occurs on this interval. We take $\bar{u} = 2$ and set

$$u = 2 + \widetilde{u},$$

Inserting this in the above equation we find the linearized equation for $\widetilde{u}(t,x)$

$$\begin{cases} \frac{\partial \widetilde{u}}{\partial t} - A'(2)\Delta \widetilde{u} = 0, \qquad x \in \Omega \\ \\ \frac{\partial}{\partial \nu} \widetilde{u} = 0 \qquad \text{on } \partial\Omega, \end{cases}$$

We set $\gamma = -A'(2) > 0$ and we look for solutions $\widetilde{u}(t,x) = e^{\lambda t} w(x)$ which are unstable, i.e., $\lambda > 0$. These are given by

$$\lambda w + \gamma \Delta w = 0,$$

and thus they stem from the Neuman 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 a possible unstable modes and thus they can be of very high frequencies. And we expect to see the mode corresponding to the largest $\lambda$, i.e., to the largest $\lambda_i$ 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 observ numerically.

Figure 7.7 gives numerical solutions to (7.14)–(7.15) 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 Section 8.9 we have introduced a relaxation system.

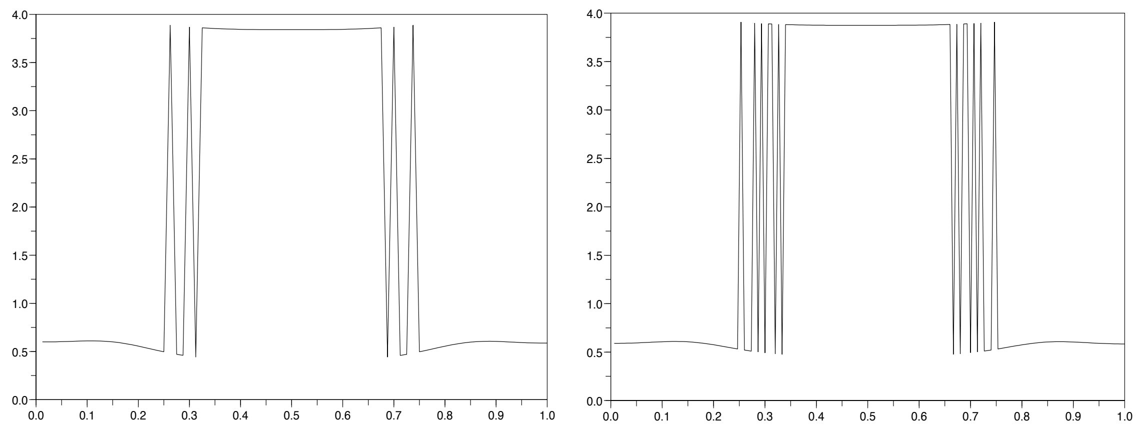


Figure 7.7: Two numerical solutions to the phase transition system (7.14)–(7.15) for (Right) 80 grid points and (Left) 150 grid points. The oscillation frequencies depend on the grid and these are not Turing patterns.

## 7.6 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 by far too complicated to be presented here and their use in biology and other applications are by far too numerous.

### 7.6.1 A cell polarity system

We take the following system from Morita and Ogawa[4]

$$\begin{cases} \frac{\partial}{\partial t}u - \sigma_1 \Delta u = -f(u) + v, & t \geq 0, \ x \in \Omega, \\ \frac{\partial}{\partial t}v - \sigma_2 \Delta v = \quad f(u) - v, & \\ u(x,t) = v(x,t) = 0 \quad \text{sur} \ \ \partial\Omega. & \end{cases} \tag{7.16}$$

We take a function $f \in C^2(\mathbb{R}^+; \mathbb{R}^+)$ that satisfies for a given value $u_c > 0$

$$f(0) = 0, \quad f'(u) > 0 \text{ for } u \in [0, u_c[, \quad -1 < f'(u) < 0 \text{ for } u > u_c, \quad f(+\infty) = 0.$$

This system is mass conservative since one can prove that

$$u(t,x) > 0, \quad v(t,x) > 0, \qquad \frac{d}{dt}\int_\Omega [u(t,x) + v(t,x)]dx = 0.$$

[4]Morita Y. and Ogawa T. Stability and bifurcation of nonconstant solutions to a reaction-diffusion system with conservation of mass, Nonlinearity 23 (2010) 1387–1411.

These properties give us the non-extinction/non-blow-up conditions.

We analyze the 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 preservs 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 (same argument fo $V$).

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 write

$$\bar{u} + \bar{v} = M^0, \qquad \bar{v} = f(\bar{u}). \tag{7.17}$$

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 (7.17). 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 which corresponds to the 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 section 7.1, this is equivalent to

$$(\sigma_1\lambda_k + f'(\bar{u}))(\sigma_2\lambda_k + 1) - f'(\bar{u}) = \sigma_1\sigma_2\lambda_k^2 + \sigma_1\lambda_k + \sigma_2 f'(\bar{u})\lambda_k < 0,$$

$$\lambda_k + \frac{1}{\sigma_2} \le \frac{|f'(\bar{u})|}{\sigma_1}.$$

This is clearly satisfied for some eigenvalues $\lambda_k$ when $\sigma_1$ is small enough; this is the same result as in Theorem 7.1.

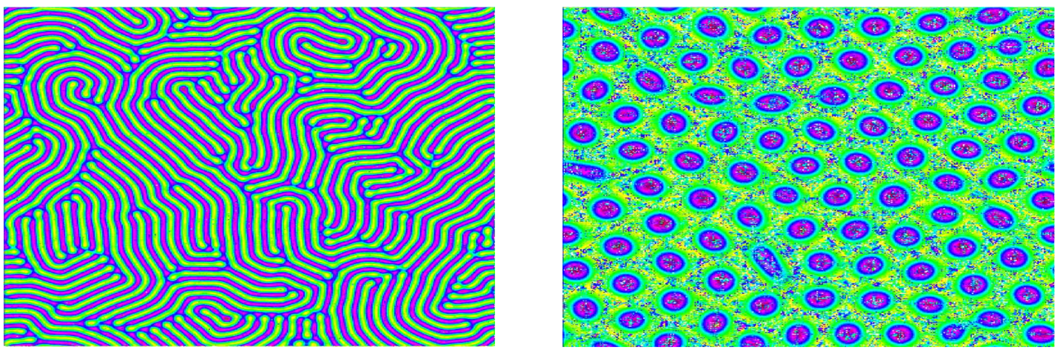

Figure 7.8: Labyrinthic and spot patterns in the CIMA reaction (7.18). The solutions have been computed with the software FreeFEM++ by S. Kaber.

### 7.6.2 The CIMA reaction

As mentioned earlier, the first experimental evidence of Turing instability was given with the CIMA (chlorite-iodide-malonic acid) chemical reaction. It was modeled by I. Lengyel and I. R. Epstein[5] who proposed the system (with $c = 1$)

$$\begin{cases} \dfrac{\partial u}{\partial t} - \sigma_u \Delta u = a - u - \dfrac{4uv}{1+u^2}, \\ \dfrac{\partial v}{\partial t} - \sigma_v \Delta v = bc\, u - \dfrac{cuv}{1+u^2}. \end{cases} \tag{7.18}$$

Here $u$ (the activator) denotes the iodide ($I^-$) concentration and $v$ (the inhibitor) the chlorite ($ClO_2^-$) concentration. Existence of steady states was analyzed [6,7].

Here we consider this system with $a > 0$, $b > 0$, $c > 0$. There is a single homogeneous steady state

$$\bar{u} = \frac{a}{4b+1}, \qquad \bar{v} = b(1 + \bar{u}^2).$$

[5] Modeling of Turing structure in the chlorite-iodide-malonic acid-starch reaction system, Science 251 (1991) 650–652.

[6] W. Ni and M. Tang. Turing patterns in the Lengyel-Epstein system for the CIMA reaction. Trans. Amer. Math. Soc 357 (2005) 3953–3969

[7] F. Yi, J. Wei and J. Shi. Diifusion-driven instability and bifurcation in the Lengyel-Epstein system reaction-diffusion system. Nonl. Anal. Real World Appl. 9 (2008) 1038–1051

The natural invariant region for solutions (that means the bounds are satisfied for all times if initially true) are given by the maximum principle

$$0 \leq u \leq a, \qquad b \leq v \leq b(1+a^2) := v_M.$$

Also solutions cannot get extinct because we can use the upper bound on $v$ to go further and find

$$u \geq u_{\min}, \qquad u_{\min}(1+\frac{4v_M}{1+u_{\min}^2}) = a.$$

(in fact we can go further and find a more restrictive invariant region, iterating the argument). These a priori bounds are just consequences of the maximum principle and we skip the derivation.

Therefore, according to our theory of Turing patterns, solution cannot get extinct or blow-up and it remains to be study the linearized operator around the steady state $(\bar{u}, \bar{v})$.

**Lemma 7.5** *The CIMA reaction system (7.18) 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, $\sigma_v$ of order one and $\sigma_u$ small enough, there will be Turing patterns.*

With the first two conditions on $b$ 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 just a condition 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 firstly need

$$4b^2\bar{u}^2 - 4b^2 - b(1+\bar{u}^2) > 0 \Longleftrightarrow \bar{u}^2 > \frac{4b+1}{4b-1}.$$

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. $\square$

### 7.6.3 The diffusive Fisher/KPP system

We can depart the quest of systems exhibiting Turing patterns with the Fisher/KPP equation (see sections 4.6 and 4.8)

$$\frac{\partial u}{\partial t} - d_u \Delta u = g(u)(1-u). \tag{7.19}$$

We recall that its main remarkable property is to exhibit traveling waves.

The natural extension to a system leads to the diffusive Fisher/KPP system already mentioned in section 4.9. It reads

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = g(u)v, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = -g(u)v. \end{cases} \tag{7.20}$$

For $d_u = d_v$, the solution $v = 1-u$ reduces (7.20) to (7.19). Therefore this system still exhibits traveling waves. It has been proved that even for $d_v \neq d_u$, the system admits monotonic traveling waves [8, 35, 36] for a power law nonlinearity $g(u) = u^n$.

Form the Turing instability alternative in section 7.1 we do not expect Turing patterns at this stage. This is why interesting examples are always a little more elaborated.

**Exercise**. Consider the steady states $(U = \gamma, V = 0)$, $\gamma > 0$ of (7.20) with $g(u) = u^n$.
1. Compute the linearized equation around this steady state.
2. In the whole space or a bounded domain with Neuman boundary condition, show that this steady state is always stable.

### 7.6.4 The Brusselator

Prigogine and Lefever[8,9] proposed an example now called the Brusselator. This is certainly the simplest system exhibiting Turing patterns; see also section 7.6.2.

Let $A > 0, B > 0$ be given positive numbers. In a finite domain $\Omega$ we consider the following $2 \star 2$ system with Neuman boundary condition

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = A - (B+1)u + u^2 v, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = Bu - u^2 v. \end{cases} \tag{7.21}$$

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.

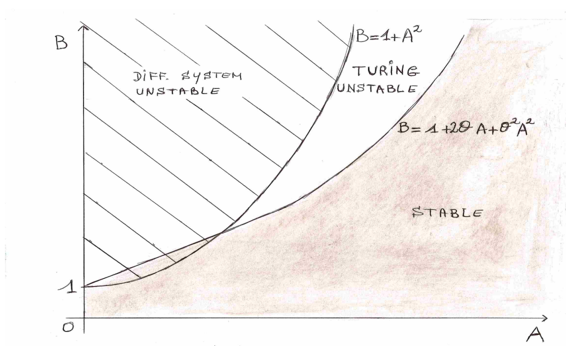

Figure 7.9: The Turing instability region in the $(A, B)$ plane.

**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 of Laplace equation with Neuman boundary condition $(\lambda_i, w_i)$. Write the condition on $A$, $B$, $d_u$, $d_v$, $\lambda_i$ which degerates an unstable mode $\lambda > 0$.
5. Show that for $\theta := \frac{d_u}{d_v} < 1$ the interval $[\Lambda_-, \Lambda_+]$ for $\lambda_i$ is not empty.

[8] Prigogine, I. and Lefever, R. Symmetry breaking instabilities in dissipative systems. II. J. Chem. Phys. **48**, 1695–1700 (1968).

[9] Nicolis G. and Prigogine, I. Self-organization in non-equilibrium systems. Wiley Interscience, New-York (1077).

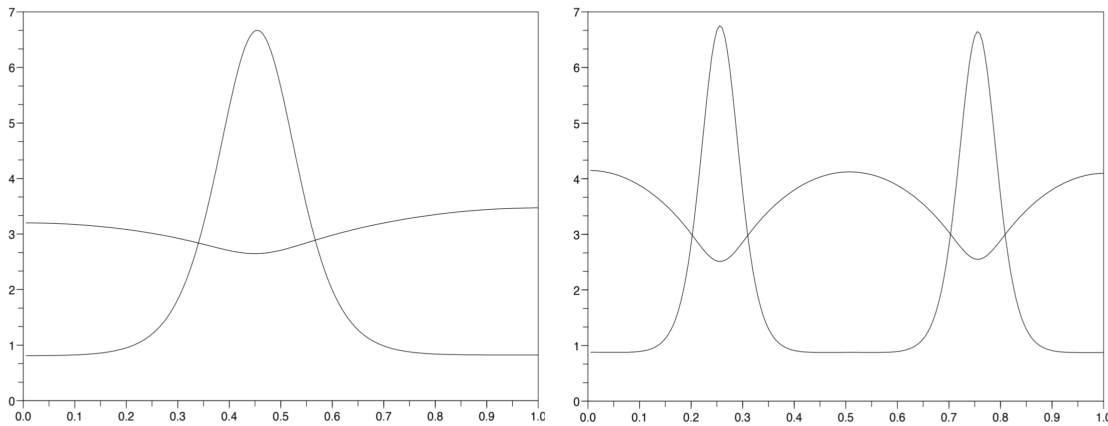


Figure 7.10: Two numerical solutions to the brusselator system (7.21) with $A = B = 2$ and 200 grid points. The choice of diffusion coefficients are (Left) $d_v = 1.$ and $d_u = 0.005$ (Right) $d_v = 0.1$ and $d_u = 0.001$. The first component $u$ exhibits one or two strong pick(s) upwards while $v$ exhibits one or two minimum(s) and has been magnified by a factor 5.

6. Show that for $\theta$ small we have $\Lambda_- \approx \frac{A^2}{d_v}$, $\Lambda_+ \approx \frac{B-1}{2d_v\theta}$. Conclude that for $d_v$ fixed and $d_u$ small, the steady state becomes unstable.

**Solution.** 2.

$$\begin{cases} \frac{\partial \widetilde{u}}{\partial t} - d_u \Delta \widetilde{u} = (B-1)\widetilde{u} + A^2 \widetilde{v}, \\ \frac{\partial \widetilde{v}}{\partial t} - d_v \Delta \widetilde{v} = -B\widetilde{u} - A^2 \widetilde{v}. \end{cases}$$

3. $det = A^2$, $tr = B - 1 - A^2$ and see Section 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 $\lambda$ 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 origin, i.e., $B > 1 + \frac{d_u}{d_v} A^2$ and also

$$(B-1)d_v - A^2 d_u > 2A\sqrt{d_u \; d_v} \Longleftrightarrow B > 1 + 2\sqrt{\theta} A + \theta A^2.$$

This is compatible with the condition of question 3. if and only if $\theta < 1$.
6. We have

$$\Lambda_\pm = \frac{1}{2d_v\theta}[B - 1 - A^2\theta \pm \sqrt{(B-1-A^2\theta)^2 - 4A^2\theta}\;].$$

The Taylor expansion for $\theta$ small reads

$$\Lambda_\pm = \frac{1}{2d_v\theta}(B-1-A^2\theta)\left[1 \pm \sqrt{1 - \frac{4A^2\theta}{(B-1-A^2\theta)^2}}\;\right]$$

$$\Lambda_{\pm} \approx \frac{1}{2d_v\theta}(B-1-A^2\theta)\left[1 \pm (1-\frac{2A^2\theta}{(B-1-A^2\theta)^2})\right]$$

and thus

$$\Lambda_{-} \approx \frac{A^2}{d_v}, \qquad \Lambda_{+} \approx \frac{B-1}{d_v\theta}.$$

For $d_v$ fixed and $\theta$ small this interval will contain eigenvalues $\lambda_i$.

The two parabolic regions in $(A, B)$ are drawn in Figure 7.9 .

### 7.6.5 Gray-Scott system (1)

Gray and Scott[10] introduced this system as a model of chemical reaction between two constituants. It differs from the Brusselator (7.21) only from the reaction terms

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u^n v - Au, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = -u^n v + B(1-v). \end{cases} \tag{7.22}$$

Again $A > 0$, $B \geq 0$ are constants (input, degradation of consituants) and $n$ is an integer, the number of molecules $u$ react with a single $v$.

The system (7.22) has he advantage over the Brusselator (7.21) that it satisfies the Turing Instability Principle in section 7.1. To explain this, we only consider the case

$$n = 2, \qquad B > 4A^2. \tag{7.23}$$

We first notice that there are three steady states; the trivial one $(U_0 = 0, V_0 = 1)$ and non-vanishing ones $(U_{\pm}, V_{\pm})$ to the Gray-Scott system, 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

$$U_{\pm} = \frac{B \pm \sqrt{B^2 - 4A^2B}}{2A}, \quad V_{\pm} = \frac{B \mp \sqrt{B^2 - 4A^2B}}{2B}. \tag{7.24}$$

It is easy (but tedious) to see that the following results hold:

**Lemma 7.6** *With the assumption (7.23), 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 (7.25) below.*

[10] Gray, P. and 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)

**Proof**. The linearized systems read

$$\begin{cases} \frac{\partial \widetilde{u}}{\partial t} - d_u \Delta \widetilde{u} = (2UV - A)\widetilde{u} + U^2 \widetilde{v}, \\ \frac{\partial \widetilde{v}}{\partial t} - d_v \Delta \widetilde{v} = -2UV\widetilde{u} - (U^2 + B)\widetilde{v}. \end{cases}$$

We begin with the trivial steady state $(U_0, V_0)$. Along with the general analysis of section 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

$$\begin{cases} \frac{\partial \widetilde{u}}{\partial t} - d_u \Delta \widetilde{u} = A\widetilde{u} + U^2 \widetilde{v} \\ \frac{\partial \widetilde{v}}{\partial t} - d_v \Delta \widetilde{v} = -2A\widetilde{u} - (U^2 + B)\widetilde{v}, \end{cases}$$

$$\mathcal{D} = A(U^2 - B) > 0, \qquad \mathcal{T} = A - B - U^2.$$

We deduce from (7.24)

$$\begin{aligned} U_\pm^2 - B &= \tfrac{B^2}{2A^2} - 2B \pm \tfrac{B}{2A^2}\sqrt{B^2 - 4A^2B} \\ &= \tfrac{B}{2A^2}\left[B - 4A^2 \pm \sqrt{B^2 - 4A^2B}\right]. \end{aligned}$$

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

$$\mathcal{T} = A - \frac{B^2}{2A^2} - \frac{B}{2A^2}\sqrt{B^2 - 4A^2B} < 0, \tag{7.25}$$

which is an additional condition to be checked. Notice that for the limiting value $B = 4A^2$ it means that $A > 1/8$. Therefore it is clearly compatible with (7.23). □

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 (7.22) 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 $A$ small enough, 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 section 4.7). For an extended study of traveling waves in Gray-Scott system, we refer to [40]

### 7.6.6 Schnakenberg system

The Schnakenberg system[11] is still another variant written as

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = C + u^2 v - Au, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = B - u^2 v. \end{cases} \tag{7.26}$$

With $C = 0$, it has been advocated by M. Ward as a simple model for spot-patterns formation and spot-splitting in the following asymptotic regime

$$\begin{cases} \dfrac{\partial u}{\partial t} - \varepsilon \Delta u = u^2 v - Au, \\ \varepsilon \dfrac{\partial v}{\partial t} - d_v \Delta v = B - \dfrac{u^2 v}{\varepsilon}. \end{cases} \tag{7.27}$$

### 7.6.7 The diffusive FitzHugh-Nagumo system

Consider again the FitzHugh-Nagumo system as already studied in Section 5.2.2, but with diffusion on both components,

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u(1-u)(u - \frac{1}{2}) - v, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = \mu u - v, \end{cases} \tag{7.28}$$

with Neuman 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 it is stable for the associated differential equation.

**Exercise**. We fix $d_v > 0$. Show that for $d_u$ small enough the steady state becomes unstable.

As already mentioned, there are many variants, one of them is

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u(1-u)(u - \alpha) - \beta uv, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = \gamma uv - \delta v(1 - v). \end{cases} \tag{7.29}$$

This makes the relation between prey-predator models and FitzHugh-Nagumo types of systems. See Section 7.7.3.

[11] Schnakenberg J., Simple chemical reactions with limit cycle behaviour. J. Theor. Biol. 81, 389–400 (1979)

### 7.6.8 Gierer-Meinhardt system

Gierer-Meinhardt [24, 37, 38] system is one of the most famous exhibiting Turing instability and Turing patterns. It can be considered as model for chemical reactions with only two reactants denoted by $u(t,x)$ and $v(t,x)$.

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - d_1\Delta u(t,x) + Au = u^p/v^q, \quad t \geq 0, \ x \in \Omega, \\ \frac{\partial}{\partial t}v(t,x) - d_2\Delta v(t,x) + Bv = u^r/v^s, \end{cases} \tag{7.30}$$

with Neuman boundary conditions.

Among this class, several authors have used the particular case with a single parameter

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - d_1\Delta u(t,x) + Au = u^2/v, \quad t \geq 0, \ x \in \Omega, \\ \frac{\partial}{\partial t}v(t,x) - d_2\Delta v(t,x) + v = u^2, \end{cases} \tag{7.31}$$

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 steady state

$$\begin{cases} -\varepsilon^2\Delta u + u = u^p, \qquad x \in \Omega, \\ \\ \frac{\partial u}{\partial \nu} = 0 \qquad on\ \partial\Omega. \end{cases} \tag{7.32}$$

Following Berestycki and Lions, there is a unique radial spike like solution $u = u_0(\frac{x}{\varepsilon})$ with

$$-\Delta u_0 + u_0 = u_0^p, \qquad x \in \mathbb{R}^d, \qquad u_0 > 0, \tag{7.33}$$

when $p < \frac{d+2}{d-2}$.

But (see Andrea Malchiodi and Montenegro) there are solutions concentrating on the boundary $\partial\Omega$ without limitation on $p$.

Also for systems there is a large litterature[12] on the numerous types of solutions, and their concentration properties in the case

$$\begin{cases} -\varepsilon^2\Delta u + u = \frac{u^2}{v}, \qquad x \in \mathbb{R}, \\ \\ -\Delta v + v = u^2. \end{cases} \tag{7.34}$$

[12] J. Wei, M. Winter. Symmetric and asymmetric mutiple clusters in a reaction-diffusion system. NoDEA 14 (2007) No 5-6, 787–823. And the references therein.

## 7.7 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.

### 7.7.1 Competing species and Turing instability

Met us come back to models of competing species as already mentioned in section 4.10. Let the coefficients $r_1$, $r_2$, $\alpha_1$ and $\alpha_2$ be positive in the system

$$\begin{cases} \frac{\partial}{\partial t}u_1 - d_1\Delta u_1 = r_1u_1(1-u_1-\alpha_2u_2), \\ \\ \frac{\partial}{\partial t}u_2 - d_2\Delta u_2 = r_2u_2(1-\alpha_1u_1-u_2). \end{cases} \tag{7.35}$$

We have seen in section 4.10 that the positive steady state $(U_1, U_2)$ is stable iff $\alpha_1 < 1$, $\alpha_2 < 1$. As stated in Theorem 7.1, to be Turing unstable, we need that one of the diagonal coefficients is positive in the linearized matrix

$$L = \begin{pmatrix} -r_1U_1 & -\alpha_2r_1U_1 \\ \\ -\alpha_1r_2U_2 & -r_2U_2 \end{pmatrix}$$

We see it is not the case. There is no activator in such systems.

### 7.7.2 Prey-predator system

In system (7.35), 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

$$tr(L) = -(r_1U_1 + r_2U_2) < 0, \qquad det(L) = r_1r_2U_1U_2(1-\alpha_1\alpha_2) > 0,$$

this steady state is stable.

Again, according to Theorem 7.1, it cannot be Turing unstable because both diagonal coefficients are negative.

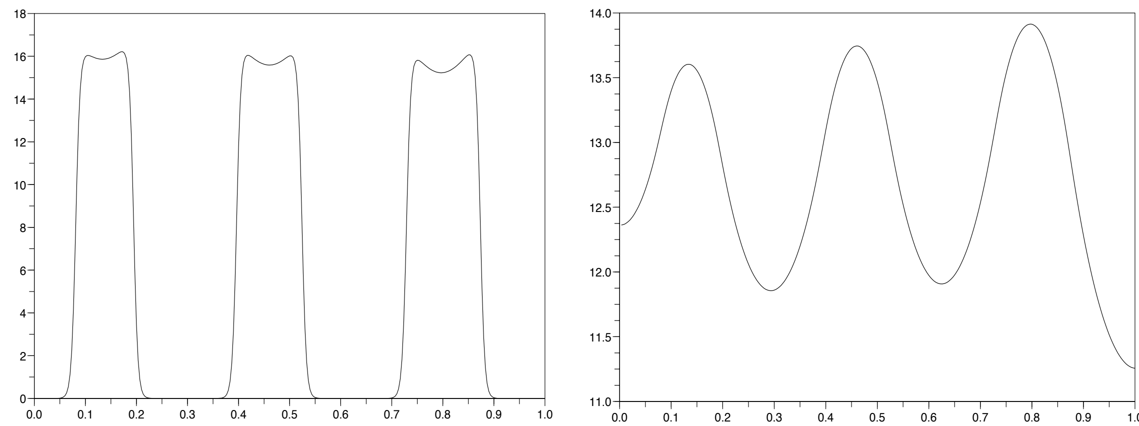


Figure 7.11: The Turing patterns created by the prey-predator system (7.36) with $\alpha = 1.8$, $\beta = .5$, $\gamma = .08$, $du = .001$ and $d_v = .6$. Left: component $u$, Right: component $v$. We have used 300 grid pointsfor the computational domain $0 \leq x \leq 1$.

### 7.7.3 Prey-predator system with Turing instability (problem)

Consider the prey-predator system (and see Section 7.6.7 for variants)

$$\begin{cases} \frac{\partial}{\partial t}u - d_u \Delta u = u(1 + u - \gamma \frac{u^2}{2} - \beta v), \\ \frac{\partial}{\partial t}v - d_v \Delta v = v(1 - v + \alpha u), \end{cases} \tag{7.36}$$

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 needed on 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 $\gamma$ small enough.

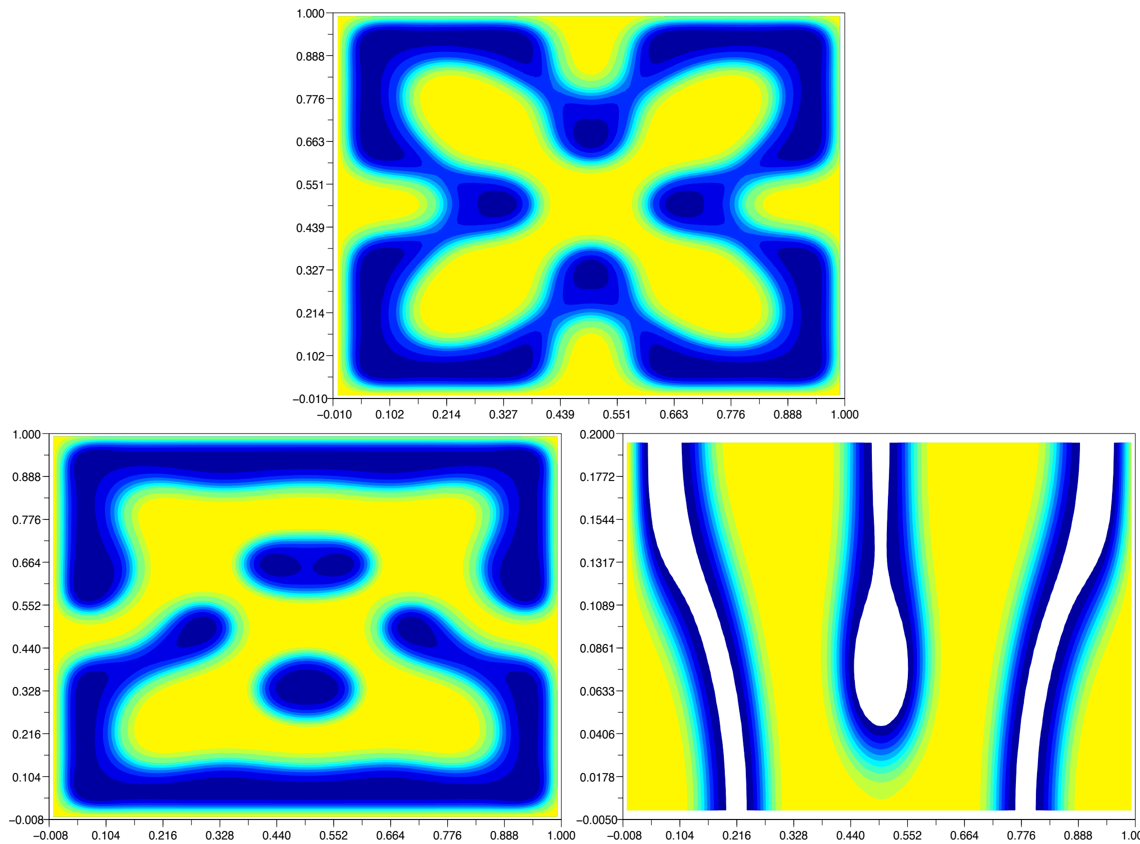


Figure 7.12: Various Turing patterns created by the prey-predator system (7.36) with $\alpha = 1.8$, $\beta = .5$, $\gamma = .08$, $du = .001$ and $d_v = .6$ in two space dimensions. We only display the component $u$. Left and Center: on a square. Right: in a rectangle $[0, 1] \times [0, .2]$.

7. State a Turing instability result on $d_u$, $d_v$ for coefficients as in 6.

Figure 7.11 shows a one dimensional numerical simulation of system (7.36) in the Turing instability regime. Figure 7.12 displays various Turing patterns in two space dimensions.

Notice also that the system has a priori bounds that follow from the maximum principle. If initially true, we have

$$\gamma \frac{u^2}{2} \leq 1 + u \quad \Longrightarrow \quad u \leq u_M := \frac{1 + \sqrt{1 - 2\gamma}}{\gamma},$$

$$v \leq v_M := 1 + u_M.$$

**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 solution positive 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 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 enough to ensure $\gamma\bar{u} < 1$ for $\gamma$ small enough. We also have to ensure $\bar{u}[1 - \alpha - \gamma\bar{u}] < 1$ (from .3) and this converges to $\bar{u}[-1-\alpha+2\alpha\beta]$ and 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 $d_u$ small enough and $d_v$ of order one, the steady state is linearly unstable.

## 7.8 Keller-Segel with growth

**Exercise**. Consider the one dimensional Keller-Segel system with growth

$$\begin{cases} u_t - u_{xx} + \chi(uv_x)_x = u(1-u), \qquad x \in \mathbb{R}, \\ -dv_{xx} + v = u. \end{cases} \tag{7.37}$$

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 on $\widehat{U}(t, k)$,

$$\widehat{U}_t + \widehat{U}\ \Lambda(k) = 0,$$

and compute $\Lambda(k)$.
4. Show that it is linearly stable under the condition $\chi \leq (1 + \sqrt{d})^2$.

**Solution** 1. is easy.
2. $U_t - U_{xx} + \chi V_{xx} \ = -U, \qquad -dV_{xx} + V = U.$
3. $\widehat{U}_t + k^2\widehat{U} + k^2\chi\widehat{V} = -\widehat{U}, \qquad -dk^2\widehat{V} + \widehat{V} = \widehat{U}.$
We can eliminate $\widehat{V}$ and find $\Lambda(k) = [k^2 + 1 - \chi\frac{k^2}{1+dk^2}]$.
4. The linear stability condition is tha all solution have the time decay $e^{-\lambda t}$ with $\lambda > 0$, in other words $\Lambda(k) > 0$. Using the shorter notation $X = k^2 \geq 0$, it reads $1 + X(d + 1 - \chi) + dX^2 \geq 0$. The analysis of the roots of this polynomial leads to 4.

# Chapter 8

# The Fokker-Planck equation

Not only diffusion but drift terms (first order derivatives) are also used in order to describe motion when a velocity field is used. The model equation is the (particular) Fokker-Planck equation for 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 this equation

• Active motion with the velocity $u = \nabla V(x)$ additionally to the brownian motion. For this reason, equation (8.1) is also called the *drift-diffusion equation*.

• Probability density of stochastic differential equations. For this reason, equation (8.1) is also called the *Kolmogorov equation*.

• Noise in particular for neurosciences.

• Chemistry as a basic model at the molecular level.

• Asymptotic limits in various formulations. An example is scattering of waves.

The main properties (formal at this stage for first two) of solutions to (8.1) are the nonnegativity principle, the 'mass' conservation and the existence of non-zero steady state,

$$n^0 \geq 0 \implies n \geq 0, \tag{8.2}$$

$$\int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} n^0(x)dx, \quad \forall t \geq 0, \tag{8.3}$$

$$\mu e^{-V(x)} \qquad \text{are steady states for all } \mu \in \mathbb{R}, \tag{8.4}$$

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 states should play a role, for instance 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 $|x| \to \infty$.

## 8.1 The relative entropy

Additionally to (8.2) and (8.3), there is another family of noticeable a priori estimates for solutions to (8.1), the so-called *relative entropy* inequalities

**Proposition 8.1** *For any convex function $H : \mathbb{R} \to \mathbb{R}$, we have*

$$\frac{d}{dt} \int_{\mathbb{R}^d} e^{-V(x)} H\left(\frac{n(t,x)}{e^{-V(x)}}\right) dx = -D_H(n|e^{-V}) \le 0,$$

$$D_H(n|e^{-V}) := \int_{\mathbb{R}^d} e^{-V} H''\left(\frac{n}{e^{-V}}\right) \left|\nabla \frac{n}{e^{-V}}\right|^2 dx.$$

A special case is $V = 0$, then we just find the usual heat equation and the usual $L^p$ estimates for $H(u) = u^p$. In general the $L^p$ estimates are true but they come with weights, 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*

$$\begin{cases} \frac{\partial}{\partial t}\underline{n} - \Delta \underline{n} - \operatorname{div}\big(\underline{n}\nabla V\big) \le 0, & t \ge 0,\ x \in \mathbb{R}^d, \\ \underline{n}(t=0,x) \le n^0(x), \end{cases} \tag{8.5}$$

*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 $H$ 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 $t \ge 0$,

$$\int_{\mathbb{R}^d} e^{-V(x)} H\left(\frac{n(t,x)}{e^{-V(x)}}\right) dx \le 0,$$

and because $H(\cdot) \ge 0$, this means that $\frac{n(t,x)}{e^{-V(x)}} \le C^0_+$ and the upper bound is proved. The lower bound is proved in a similar way. $\square$

**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 (smooth enough) 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 $x$. $\square$

**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.

## 8.2 Weak solutions

As we did it in Chapter 3, we define weak solution to (8.1) by testing against functions $\Phi \in \mathcal{D}(\mathbb{R}^+ \times \mathbb{R}^d)$

$$\int_0^\infty \int_{\mathbb{R}^d} n(t,x)\left[-\frac{\partial \Phi}{\partial t} - \Delta\Phi + \nabla V.\nabla\Phi\right] dx\, dt = \int_{\mathbb{R}^d} n^0(x)\Phi(0,x)dx. \tag{8.6}$$

We see that this makes sense under different assumptions on $V$. 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 natural in view of mass conservation.

Another option is to use, as we did it for the relative entropy structure, the alternative formulation

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \mathrm{div}\big(e^{-V(x)}\nabla(n(t,x)e^{V(x)})\big) = 0, \qquad t \ge 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.7}$$

This leads to another possible weak formulation

$$\int_0^\infty \int_{\mathbb{R}^d} n(t,x)\left[-\frac{\partial \Phi}{\partial t} - e^{V(x)}\mathrm{div}\big(e^{-V(x)}\nabla\Phi\big)\right] dx\, dt = \int_{\mathbb{R}^d} n^0(x)\Phi(0,x)dx.$$

which is not very different from (8.6).

When applying the Lax-Milgram theory for steady states, the two formulations are however very different. The direct formulation leads to use the scalar product (definiteness should comme from zeroth order term for instance)

$$((n,\Phi))_1 = \int_{\mathbb{R}^d} \nabla n(x).\nabla\Phi(x)dx + \int_{\mathbb{R}^d} n(x)\nabla\Phi(x).\nabla V dx$$

The modified formulation leads to the scalar product (we use the test function $\Phi(x) = \phi(x)e^{V(x)}$)

$$((n,\phi))_2 = \int_{\mathbb{R}^d} \nabla(n(x)e^{V(x)}).\nabla(\phi(x)e^{V(x)})e^{-V(x)}dx = \int_{\mathbb{R}^d} \nabla\widetilde{n}(x).\nabla\Phi(x)e^{-V(x)}dx.$$

This a self-adjoint scalar product on the Hilbert space $H^1(e^{-V(x)}dx)$ with definiteness directly related to the Poincaré inequality, see section**??**??.

## 8.3 The deterministic case

The case without diffusion makes sense and is called the *transport equation.* It enters in the class of hyperbolic equations and it is useful to first consider a variant.

**The strong (conservative form).** This refers to the equation

$$\begin{cases} -\frac{\partial}{\partial t}u(t,x) - U(t,x).\nabla u = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ u(t=0,x) = u^0(x) \in C^1(\mathbb{R}^d), \end{cases} \tag{8.8}$$

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 to the Ordinary Differential System*

$$\begin{cases} \frac{dX(t;x^0)}{dt} = U(t, X(t;x^0)), \\ X(0) = x^0 \in \mathbb{R}^d. \end{cases} \tag{8.9}$$

are constant along the characteristics, which are defined as the solutions to (8.9).

**Lemma 8.5** *The solution to* (8.8) *are given through the formula*

$$u(t, X(t;x^0)) = u^0(x^0) \qquad \forall t \geq 0,\ \forall x \in \mathbb{R}^d.$$

*In other words, solutions are constant along the characteristics.*

**Proof**. For a $C^1$ function one can write

$$\begin{aligned} \frac{d}{dt}u(t,X(t;x^0)) &= \frac{\partial}{\partial t}u(t,X(t;x^0)) + \dot{X}(t;x^0).\nabla u(t,X(t;x^0)) \\ &= \frac{\partial}{\partial t}u(t,X(t;x^0)) + U\big(X(t;x^0)\big).\nabla u(t,X(t;x^0)). \end{aligned}$$

This derivative vanishes if and only if the transport equation (8.8) is satisfied (and the Cauchy-Lipschitz theorem tells us that, when $x^0$ cover $\mathbb{R}^d$, then $X(t;x^0)$ alsocovers $\mathbb{R}^d$. □

**The divergence (conservative) form.** This is the equation

$$\begin{cases} \frac{\partial}{\partial t}n(t,x) + \text{div}\big(n(t,x)U(t,x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.10}$$

**Lemma 8.6** *For* $n^0(x) := \sum_{k=1}^{K} \rho_k^0 \delta(x - x_k^0)$*, the solution to* (8.10) *is given by the formula*

$$n(t,x) = \sum_{k=1}^{K} \rho_k^0 \delta\big(x - X(t; x_k^0)\big).$$

For this reason we see that the population density is transported by the flow field $U$. We also see that $L^1$ is a natural space for $n^0 \in L^1$ by mass conservation. The general formula for the solution not as simple for Dirac mass 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

$$n(t, X(t,y)) \exp \int_0^t \mathrm{div} U\,(s, X(s;y)ds = n^0(y) \qquad \forall t \geq 0,\ \forall y \in \mathbb{R}^d.$$

## 8.4 The complete Fokker-Planck equation

The complete Fokker-Planck equation (also called Kolmogorov equation in the theory of Markov processes) is given by

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i\, \partial x_j} \big(B_{ij}(t,x) n(t,x)\big) + \mathrm{div}\big(n(t,x) U(t,x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.11}$$

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 non-negative symmetric diffusion matrix. In other words, it is always assumed to satisfy, for some $\nu \geq 0$,

$$\sum_{i,j=1}^{d} B_{ij}(t,x) \xi_i \xi_j \geq \nu |\xi|^2 \qquad \forall \xi \in \mathbb{R}^d.$$

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 $N$ to (8.1) that is

$$-\frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i\, \partial x_j} \big(B_{ij}(x) N(x)\big) + \mathrm{div}\big(N(x) U(x)\big) = 0, \qquad 0,\ x \in \mathbb{R}^d, \qquad N(x) > 0. \tag{8.12}$$

The existence of solutions depends heavily on the coefficients $(B, U)$ but a typical example is as before

$$\frac{1}{2}B = I \quad \text{(Idendity matrix)}, \qquad U(x) = -\nabla V(x), \qquad N(x) = e^{-V(x)}.$$

Then, we 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, just calculate successively the equation on $u(t,x) = \frac{n(t,x)}{N(x)}$, then on $H\big(u(t,x)\big)$, and then on $NH\big(u(t,x)\big)$. It is tedious but it works.

There are many examples of nonlinear Fokker-Planck equations arising in biology and we give examples later on. 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 they play a central role is the connection with brownian motion and Stochastic Differential Equations. This material is introduced later on.

## 8.5 Stochastic Differential Equations

For a given smooth enough vector field $U \in \mathbb{R}^d$ and a matrix $\sigma(t,x) \in M_{d,p}$, one can build the solution to the Itô Stochastic Differential Equation

$$\begin{cases} dX(t) = U\big(t, X(t)\big)dt + \sigma\big(t, X(t)\big)dW(t), \\ X(0) = X^0 \in \mathbb{R}^d \quad \text{(a random vector)}, \end{cases} \tag{8.13}$$

with $W(t) = \big(W^1(t), ...W^p(t)\big)$, $p$ independent brownian motions.

The numerical construction mimicks the one of the brownian motion in section 1.4 and we use the same notations. It is to define the Euler scheme (here we calculate with $d = p = 1$ but the reader can extend it easily)

$$X^{k+1} = X^k + \Delta t\, U\big(t^k, X^k\big) + \sqrt{\Delta t}\, \sigma\big(t^k, X^k\big) Y^k. \tag{8.14}$$

Because the random variable $Y^k$ is independent of $X^k$ and $\mathbb{E}[Y^k] = 0$, we have

$$\mathbb{E}\left[X^{k+1} - X^k\right] = \Delta t \mathbb{E}\big[U\big(t^k, X^k\big)\big], \tag{8.15}$$

$$
\begin{aligned}
\mathbb{E}\left[\left(X^{k+1}-X^k\right)^2\right] &= \mathbb{E}\left[\Delta t^2 U^2\left(t^k,X^k\right)+2\sqrt{\Delta t}U\left(t^k,X^k\right)\sigma\left(t^k,X^k\right)Y^k+\Delta t\left|\sigma\left(t^k,X^k\right)Y^k\right|^2\right] \\
&= \Delta t\,\mathbb{E}\left[\sigma^2\left(t^k,X^k\right)\right]\mathbb{E}\left[\left(Y^k\right)^2\right]+O(\Delta t^2) \\
&= \Delta t\,\mathbb{E}\left[\sigma^2\left(t^k,X^k\right)\right]+O(\Delta t^2)
\end{aligned}
$$

Except when $\sigma \equiv 0$, this scales like the brownian motion.

The type of aproximation scheme used here is very important and, in opposition to the deterministic case, changing it also changes the limit. The Stratonovich convention is an example and the notion is denoted as

$$
\begin{cases} dX(t) = U\big(t,X(t)\big)dt+\sigma\big(t,X(t)\big)\circ dW(t), \\ X(0)=X^0\in\mathbb{R}^d \quad \text{(a random vector).} \end{cases} \tag{8.16}
$$

The Stratonovich SDE corresponds to the semi-implicit approximation

$$
X^{k+1} = X^k+\Delta t\,U\big(t^k,X^k\big)+\sqrt{\Delta t}\,\sigma\big(t^k,\frac{X^k+X^{k+1}}{2}\big)Y^k, \tag{8.17}
$$

which we may approximate as

$$
\begin{aligned}
X^{k+1} &\approx X^k+\Delta t\,U\big(t^k,X^k\big)+\sqrt{\Delta t}\,\Big[\sigma\big(t^k,X^k\big)+\tfrac{1}{2}D\sigma\big(t^k,X^k\big)(X^{k+1}-X^k)\Big]Y^k \\
&\approx X^k+\Delta t\,U\big(t^k,X^k\big)+\tfrac{\Delta t}{2}D\sigma\big(t^k,X^k\big)\sigma\big(t,X^k\big)\big(Y^k\big)^2+\sqrt{\Delta t}\,\sigma\big(t^k,X^k\big)Y^k+O(\Delta t^{3/2}).
\end{aligned}
$$

This means that

$$
\mathbb{E}\left[X^{k+1}-X^k\right] = \Delta t\mathbb{E}\big[U\big(t^k,X^k\big)\big]+\frac{\Delta t}{2}\mathbb{E}\big[D\sigma\big(t^k,X^k\big)\sigma\big(t^k,X^k\big)\big)\big], \tag{8.18}
$$

in other words, one cannot take the expectation as simply as for Itō-Doeblin SDE.

Because $\mathbb{E}\left[(Y^k)^3\right]=0$, we also find that

$$
\mathbb{E}\left[\left(X^{k+1}-X^k\right)^2\right] = \Delta t\,\mathbb{E}\big[\sigma^2\big(t^k,X^k\big)\big]+O(\Delta t^2).
$$

It is remarkable that the Stratonovich semi-implicit scheme leads to the same two leading expectations as the Itō-Dœblin method with the drift $U$ changed in $U-\frac{1}{2}\sigma'\sigma$; in fact in the limit $\Delta t\to 0$ the two constructions are equivalent with this modification on the drift. This is to say that the term $\big(Y^k\big)^2$ is worth 1 in the limit.

## 8.6 The Itō-Dœblin formula

An important tool in the theory of SDEs is the Itō-Dœblin formula that gives the equation satisfied by the random variable $u(t,X(t))$, when $u\in C^2(\mathbb{R}^{d+1};\mathbb{R})$,

$$
\begin{aligned}
du(t,X(t)) &= \Big[\tfrac{\partial u(t,X(t))}{\partial t}+U\big(t,X(t)\big).Du\big(t,X(t)\big)+\tfrac{1}{2}B\big(t,X(t)\big).D^2u\big(t,X(t)\big)\Big]\,dt \\
&\quad +\sigma\big(t,X(t)\big).Du\big(t,X(t)\big).dW(t)
\end{aligned} \tag{8.19}
$$

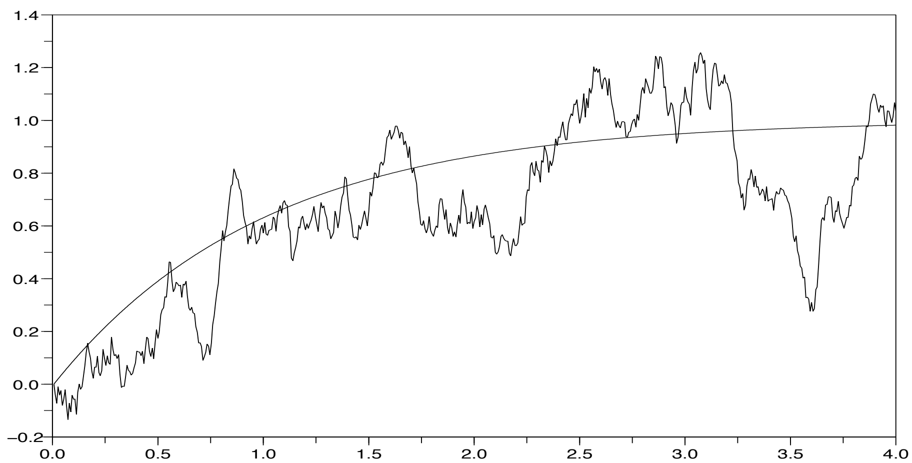

Figure 8.1: Deterministic solution ($\sigma = 0$) and a path solution ($\sigma = \frac{1}{2}$) to the Itō-Doeblin SDE (8.14) for the drift $U(x) = 1 - x$.

with

$$B(t,x) = \frac{1}{2}\sigma(t,x).\sigma^t(t,x) \qquad (\sigma^t \text{ denotes the transposed matrix}). \tag{8.20}$$

In other words, the chain rule does not apply to SDEs as it applies to ODEs ($\sigma(t,x) = 0$) and it gives an extra drift, namely the term $B\big(t, X(t)\big).D^2u\big(t, X(t)\big)$.

This formula can be derived from the approxumation (8.14). Using Taylor expansion, we find

$$\begin{aligned} u(t^{k+1}, X^{k+1}) &= u(t^k, X^{k+1}) + \Delta t \tfrac{\partial u(t^k, X^{k+1})}{\partial t} + O(\Delta t^2) \\ &= u(t^k, X^{k+1}) + \Delta t \tfrac{\partial u(t^k, X^k)}{\partial t} + O(\Delta t^{3/2}). \end{aligned}$$

Therefore

$$\begin{aligned} u(t^{k+1}, X^{k+1}) &= u(t^k, X^k) + \Delta t \tfrac{\partial u(t^k, X^k)}{\partial t} + O(\Delta t^{3/2}) \\ &+ \big[\Delta t U(t^k, X^k) + \sqrt{\Delta t}\ \sigma\big(t^k, X^k\big)Y^k\big].Du(t^k, X^k) \\ &+ \tfrac{1}{2}\Delta t \sigma\big(t^k, X^k\big)^2\big(Y^k\big)^2 D^2u(t^k, X^k). \end{aligned}$$

As we already saw it for the Stratonovich model, the term $\big(Y^k\big)^2$ is worth 1 in the limit $\Delta t \to 0$ and we see that this is the discrete version of (8.19).

In the case of Stratonovich convention, one can use the chain rule as in the deterministic case

$$du(t, X(t)) = \left[\frac{\partial u(t, X(t))}{\partial t} + U\big(t, X(t)\big).Du\big(t, X(t)\big)\right]\Delta t + \sigma\big(t, X(t)\big).Du\big(t, X(t)\big) \circ dW(t). \tag{8.21}$$

To see this, we can redo the discrete version, and to simplify, use a function of $X$ only,

$$u(X^{k+1}) = u(X^k) \quad +Du(X^k)[\Delta t\, U\big(t^k, X^k\big) + \sqrt{\Delta t}\, \sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)Y^k]$$
$$+\tfrac{\Delta t}{2} D^2 u(X^k)\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)^2 (Y^k)^2 + O(\Delta t^{3/2})$$

which we may 'center' to follow the semi-implicit rule

$$u(X^{k+1}) = u(X^k) \quad +\Delta t\, Du(X^k)U\big(t^k, X^k\big) + \sqrt{\Delta t}\, Du\big(\tfrac{X^k+X^{k+1}}{2}\big)\sqrt{\Delta t}\, \sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)Y^k$$
$$-\tfrac{\sqrt{\Delta t}}{2} D^2 u(X^k)(X^{k+1} - X^k)\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)^2 Y^k$$
$$+\tfrac{\Delta t}{2} D^2 u(X^k)\sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)^2 (Y^k)^2 + O(\Delta t^{3/2})$$

and because the dominant term in $X^{k+1} - X^k$ is $\sqrt{\Delta t}\, \sigma\big(\tfrac{X^k+X^{k+1}}{2}\big)Y^k$, 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 (8.21).

## 8.7 The Kolmogorov equation

To go further we recall that

**Definition 8.8** *The probability density $n(x)$ of a random variable $X$ is defined as*

$$\int u(x)n(x)dx = \mathbb{E}\big[u(X(\omega))\big].$$

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-Dœblin formula that $n$ satisfies the Fokker-Planck equation (8.1)which comes naturally with the 'mass conservation' property because, for a probability density, we have $\int_{\mathbb{R}^d} n(t,x)dx = 1$. To see this we write, taking the expectation in (8.19), that for any smooth function $u(t,x)$ it holds

$$\frac{d}{dt}\mathbb{E}\big[u(t, X(t)\big] = \mathbb{E}\left[\frac{\partial u(t, X(t))}{\partial t} + U\big(t, X(t)\big).Du\big(t, X(t)\big) + \frac{1}{2}B\big(t, X(t)\big).D^2 u\big(t, X(t)\big)\right].$$

Using the definition of the probability density $n(t,x)$ of the process $X(t)$, we find

$$\frac{d}{dt}\int u(t,x)n(t,x)dx = \int \frac{\partial u(t,x)}{\partial t} n(t,x)dx + \int \big[U(t,x).Du(t,x) + \frac{1}{2}B(t,x).D^2 u(t,x)\big]n(t,x)dx.$$

Because

$$\frac{d}{dt}\int u(t,x)n(t,x)dx = \int \frac{\partial u(t,x)}{\partial t} n(t,x)dx + \int u(t,x)\frac{\partial n(t,x)}{\partial t}dx,$$

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

$$0 = \int u(t,x)\left[-\frac{\partial n(t,x)}{\partial t} - \text{div}[U(t,x).n(t,x)] + D^2[\frac{1}{2}B(t,x).n(t,x)]\right]dx.$$

Because this holds true for any function $u(t,x)$, we conclude that

$$-\frac{\partial n(t,x)}{\partial t} - \text{div}[U(t,x).n(t,x)] + D^2[\frac{1}{2}B(t,x).n(t,x)] = 0,$$

that is the general Fokker-Planck equation.

We can use the same derivation for the Euler discrete scheme (8.14) and write for all smooth functions $u(x)$ that, still with $N$ the normal law,

$$u\big(X^{k+1}\big) = u\Big(X^k + \Delta t\ U\big(t^k, X^k\big) + \sqrt{\Delta t}\ \sigma\big(t^k, X^k\big)Y^k\Big),$$

$$\int u(x)n^{k+1}(x)dx = \int\int u\Big(x + \Delta t U(t^k,x) + \sqrt{\Delta t}\ \sigma(t^k,x)y\Big)\ n^k(x)N(y)dxdy.$$

We can hardly get an equation on $n^k$ from this formula but we canuse again Taylor formula to get the approximation

$$\int u(x)n^{k+1}(x)dx = \int\int \Big[u(x) + \Delta t U(t^k,x).Du(x) + \sqrt{\Delta t}\ \sigma\big(t^k,x)y.Du(x) + \frac{\Delta t}{2}\sigma(t^k,x)^2y^2\Big]\ n^k(x)N(y)dxdy + O(\Delta t^{3/2}),$$

$$\begin{aligned}\int u(x)n^{k+1}(x)dx &= \int \big[u(x) + \Delta t U(t^k,x).Du(x) + \tfrac{\Delta t}{2}B(t^k,x)\big]\ n^k(x)dx + O(\Delta t^{3/2})\\ &= \int u(x)\big[n^k(x) - \Delta t\ \text{div}[U(t^k,x)n^k(x)] + \tfrac{\Delta t}{2}D^2[B(t^k,x)n^k(x)]\big]\ dx + O(\Delta t^{3/2}).\end{aligned}$$

Because this holds true for all smooth function $u$, it means that

$$n^{k+1}(x) = n^k(x) - \Delta t\ \text{div}[U(t^k,x)n^k(x)] + \frac{\Delta t}{2}D^2[B(t^k,x)n^k(x)] + O(\Delta t^{3/2}).$$

As $\Delta t$ vanishes, we recover the general Fokker-Planck equation

$$-\frac{\partial n(t,x)}{\partial t} - \text{div}[U(t,x).n(t,x)] + D^2[\frac{1}{2}B(t,x).n(t,x)] = 0.$$

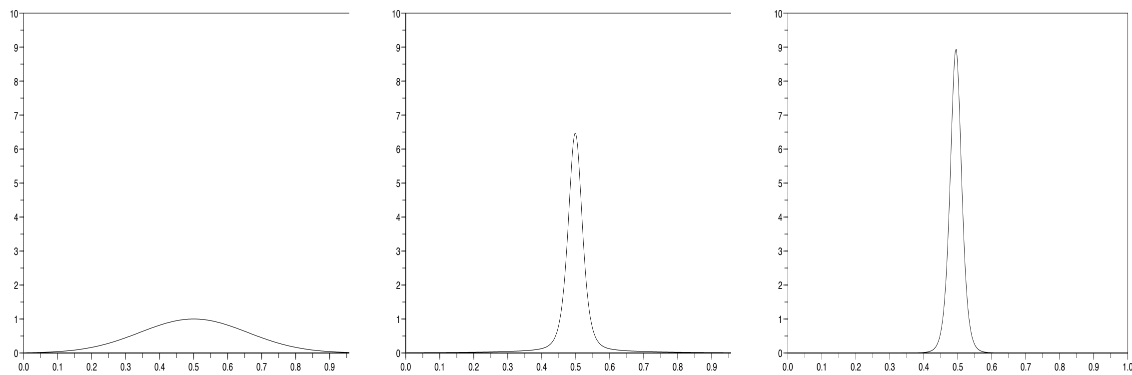

Figure 8.2: A numerical solution to (8.22) at three different times for an atractive interaction kernel $K$. Such models have the property to create high concentrations (aggregations).

## 8.8 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 with randomly with an oriented drift. The drift can arise from the collective behaviour of the individuals that creates a signal $S(t,x)$. Then one arrives to a nonlinear version of the Fokker-Planck equation

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - \Delta n(t,x) + \operatorname{div}\big(n(t,x)\nabla S(t,x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ Si(t,x) = \int_{\mathbb{R}^d} K(x-y)n(t,y)dy, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.22}$$

The convolution kernel $K(\cdot)$ describes the long range effect of an individual located at $y$ on another individual located at $x$, creating the interaction potential (signal) $S(x)$. 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 an homogeneous and isotropic medium, the kernel satifies $K(x) = \bar{K}(|x|)$. One distinguishes the attractive movement $\bar{K}(\cdot) \geq 0$, $\bar{K}'(\cdot) \leq 0$ and the case $\bar{K}(\cdot) \leq 0$, $\bar{K}'(\cdot) \geq 0$ for repulsive movement (in physics the former corresponds to newtonian gravitational forces, the later to coulombic electric forces). This can be seen from the exercise below. Figure 8.2 depicts the numerical solution to (8.22) in the attractive case. When the total density is high enough the population has tendency to aggregate and form a spike solution (see Section 5.1).

The Keller-Segel system [30] 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 the gradient of a quantity depending on the other individuals. For certain cells, this is a well documented behavior called *chemotaxis*; each cell emits a chemoattractant, i.e., molecule which diffuses in the medium and attract the other cells. They react by a biased random motion in the direction of higher concentrations of this chemoattractant. The Keller-Segel system corresponds to a singular kernel $K(\cdot)$ (the fundamental solution to the Laplace equation). Then, the solution to (8.22) can concentrate in finite time as a Dirac mass, see section 6.3.

**Exercise**. Assume that $K(x) = \bar{K}(|x|)$.
1. Derive formally the free energy for the solutions to (8.22)

$$\frac{d}{dt}\int_{\mathbb{R}^d} \big[n(t,x)\ln n(t,x) - \frac{1}{2}n(t,x)S(t,x)\big]dx := -D(t) \leq$$

and compute $D(t)$.
2. Compute $E(t)$ for the dynamics of second moment

$$\frac{d}{dt}\int_{\mathbb{R}^d} \frac{|x|^2}{2} n(t,x)dx = E(t).$$

3. Interpret these relations in terms of attractive or repulsive kernels.
Solution: $D(t) = \int_{\mathbb{R}^d} n|\nabla(S+\ln n)|^2 dx$.
$E(t) = d\int_{\mathbb{R}^d} n^0 + \frac{1}{2}\int_{\mathbb{R}^d\times\mathbb{R}^d} |x-y|\bar{K}'(|x-y|)n(t,x)n(t,y)dx\,dy$

## 8.9 Unoriented collective motion

Movement can also be completely passive, by this we mean just a brownian motion with variable intensity (and thus of zero mean), and nevertheless it can give interesting patterns. This is the case when $U \equiv 0$ in (8.13) 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 like (or need) the rest of the population, then $\Sigma'(\cdot) \leq 0$ which means that the higher is the population, the lower is the movement. When the individuals do not like high concentrations we take $\Sigma'(\cdot) \geq 0$. The Fokker-Planck equation reduces to the parabolic equation for the density

$$\begin{cases} \frac{\partial}{\partial t}n(t,x) - \Delta A\big(n(t,x)\big) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ A(n) = n\Sigma(n)^2, \\ n(t=0,x) = n^0(x). \end{cases} \tag{8.23}$$

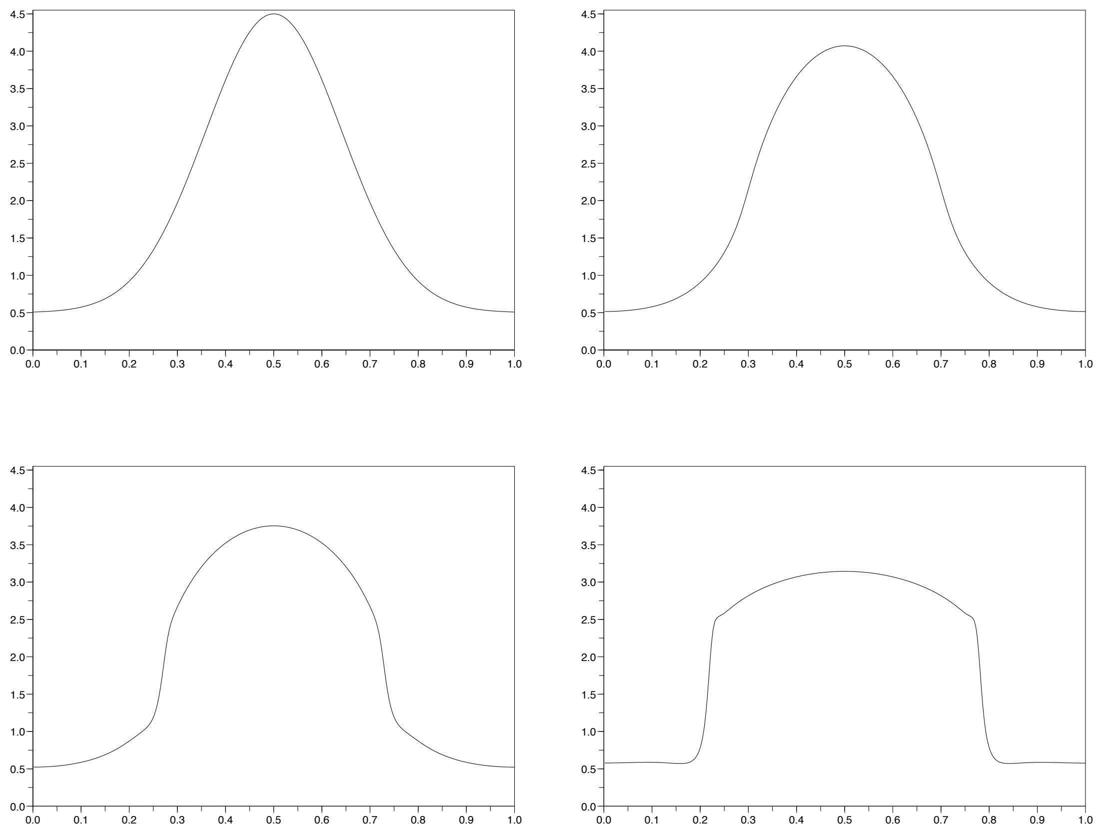

Figure 8.3: A numerical solution $n(t,x)$ to (8.23) at four different times when $A(n)$ has a decreasing region for $1 \leq n \leq 2$. Top left, the initial data. Bottom right, the last time (the steady state is composed of two constant states separated by two discontinuities).

In Figure 8.3, we present the numerical solutions to a relaxation system close to (8.23):

$$\begin{cases} \frac{\partial}{\partial t} n_\varepsilon(t,x) - \Delta[\Sigma^2\big(m_\varepsilon(t,x)\big) n_\varepsilon(t,x)] = 0, \qquad t \geq 0, \ x \in (0,1), \\ -\varepsilon \Delta m_\varepsilon(t,x) + m_\varepsilon(t,x) = n_\varepsilon(t,x), \end{cases} \tag{8.24}$$

together with Neumann boundary conditions on 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 $A'(n) \leq$ for $1 \leq n \leq 2$. This is an unstable region and that creates discontinuities. The total number constraint makes that a part of the population has to remain at a low level of density.

**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?

**Exercise**. Perform a numerical simulation of the system (8.24) and use a decreasing function $\Sigma$. Compare with the results in Figure 8.3.

The case of two species leads to a similar derivation. Each brownian motion has an intensity which depends on the densities $n_1$ and $n_2$ of the two species and leads to a Fokker-Planck equation. We arrive to a coupled system

$$\begin{cases} \frac{\partial}{\partial t} n_1(t,x) - \Delta[n_1\, a_1\big(n_1(t,x), n_2(t,x)\big)] = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} n_2(t,x) - \Delta[n_2\, a_2\big(n_1(t,x), n_2(t,x)\big)] = 0. \end{cases} \tag{8.25}$$

In such models where the $a_i$ depend on $n_j$, second order derivatives of $n_j$ arise in the equation for $n_1$ and, thus, are called *cross- diffusions*.

# Chapter 9

# From scattering to the Fokker-Planck equation

The scattering models are integral equations closely related to the Fokker-Planck equations but simpler to analyze. They come from physics (neutrons transport, wave scattering) but also from adaptive evolution to represent mutations of organisms during reproduction.

## 9.1 The scattering equation

### The integral model

We depart from the simple ordinary differential equation (in infinite dimension)

$$\frac{\partial}{\partial t}n(t,x) + k(x)n(t,x) = \int_{\mathbb{R}^d} K(y, x-y)n(t,y)dy, \tag{9.1}$$

together with an initial data $n^0 \in L^1(\mathbb{R}^d)$. We will use the assumption,

$$K(y,z) \geq 0, \qquad k(y) := \int_{\mathbb{R}^d} K(y,z)dz \in L^\infty(\mathbb{R}^d). \tag{9.2}$$

This integral model shares properties with the Fokker-Planck equation

$$n^0 \geq 0 \implies n \geq 0, \tag{9.3}$$

$$\int_{\mathbb{R}^d} n(t,x)dx = \int_{\mathbb{R}^d} n^0(x)dx, \quad \forall t \geq 0, \tag{9.4}$$

$$\int_{\mathbb{R}^d} |n(t,x)|dx \leq \int_{\mathbb{R}^d} |n^0(x)|dx, \quad \forall t \geq 0. \tag{9.5}$$

However there are not always simple formulas for the steady state.

## Existence of solutions to the scattering equation

The existence and uniqueness of solutions to (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 s a unique solution $n \in C\big(\mathbb{R}^+; L^1(\mathbb{R}^d)\big)$ to* (9.1) *and the properties* (9.3)*,* (9.4) *and* (9.5) *hold true.*

**Proof**. We first prove that the linear operator $n \mapsto k(x)n(x) - \int_{\mathbb{R}^d} K(y, x-y)n(t,y)dy$ is Lipschitz continous from $L^1$ into $L^1$. That is because

$$\|k(x)n(x)\|_{L^1(\mathbb{R}^d)} \leq \|k\|_{L^\infty(\mathbb{R}^d)} \|n(x)\|_{L^1(\mathbb{R}^d)},$$

$$\| \int_{\mathbb{R}^d} K(y, x-y)n(t,y)dy\|_{L^1(\mathbb{R}^d)} \leq \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} K(y,x-y)|n(t,y)|dy\, dx \leq \|k\|_{L^\infty(\mathbb{R}^d)}\|n(x)\|_{L^1(\mathbb{R}^d)}.$$

Then, we may apply the Cauchy-Lipschitz Theorem; in the Banach space $L^1(\mathbb{R}^d)$ a Lipschitz continuous differential equation admits 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 (9.4).

To include the sign, we introduce a family $H_\delta(\cdot)$ of smooth, non-decreasing and convex functions such that $H'_\delta(\cdot) \leq 1$ and $H_\delta(\cdot) \nearrow H(\cdot) = sign_+(\cdot)$. We have

$$\begin{aligned} \tfrac{\partial}{\partial t} H_\delta(n(t,x)) + k(x)H'_\delta(n(t,x))n(t,x) \quad &= H'_\delta(n(t,x)) \textstyle\int_{\mathbb{R}^d} K(y,x-y)n(t,y)dy \\ &\leq \textstyle\int_{\mathbb{R}^d} K(y,x-y)n_+(t,y)dy. \end{aligned}$$

Therefore, in the limit $\delta \to 0$,

$$\frac{\partial}{\partial t} n_+(t,x)dx + k(x)n_+(t,x) \leq \int_{\mathbb{R}^d} K(y,x-y)n_+(t,y)dy,$$

and

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_+(t,x)dx \leq 0.$$

Therefore if $n^0$ is nonpositive, it remains nonpositive and, applying to $-n^0$ we find (9.3).

The $L^1$ contraction (9.5) follows with the combination $-n + 2n_+ = |n|$. $\square$

## 9.2 The relative entropy

As all linear problems that satisfy a positivity principle, the scattering equation admits a family of relative entropy. We assume that the equation admits 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 $k$ and $K$ as

$$k(x) \equiv 1, \qquad K(y, x-y) = N(x).$$

Another larger class of examples is to choose, still being given $N(x) > 0$ with $\int_{\mathbb{R}^d} N = 1$ and a symmetric kernel $\widetilde{K}(x,y) = \widetilde{K}(y,x) > 0$,

$$K(y, x-y) = \frac{\widetilde{K}(x,y)}{N(y)}, \qquad k(y) := \int \frac{\widetilde{K}(x,y)}{N(y)} dx \Longleftrightarrow k(x)N(x) = \int \widetilde{K}(y,x)dy = \int \widetilde{K}(x,y)dy.$$

**Theorem 9.2 (Relative entropy for the scattering equation)** *For all convex function $H(\cdot)$, one has*

$$\frac{d}{dt}\int_{\mathbb{R}^d} N(x)H\left(\frac{n(t,x)}{N(x)}\right) := -D_H^{sc}(n|N) \leq 0,$$

$$D_H^{sc}(n|N) = \int_{\mathbb{R}^d\times\mathbb{R}^d} K(y,x-y)N(y)\left[H\left(\frac{n(t,y)}{N(y)}\right) - H\left(\frac{n(t,x)}{N(x)}\right) + H'\left(\frac{n(t,x)}{N(x)}\right)\left(\frac{n(t,x)}{N(x)} - \frac{n(t,y)}{N(y)}\right)\right] dx\, dy.$$

**Proof**. Left to the reader (see [45]). □

**Corollary 9.3** *Assume that $n^0 \leq C^0 N$, then for all $t \geq 0$,*

$$n(t,x) \leq C^0 N.$$

**Exercise**. The aim of this exercise is to give a class of kernels for which a positive steady state $N(x)$ exists in (9.6). We give, for $i = 1, 2, ..., I$ 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 set

$$k(x)=\sum_{i=1}^{I}Q_i(x),\qquad K(y,x-y)=\sum_{i=1}^{I}P_i(x)Q_i(y).$$

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 iff $\sum_{j=1}^{I}A_{ij}\alpha_j=\alpha_i$, $\forall i=1,..,I$ with the matrix with positive coefficients

$$A_{ij}=\int_{\mathbb{R}^d}\frac{P_j(y)}{k(y)}Q_i(y)dy>0.$$

2. Using Perron-Froebenius theorem show 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 (8.10) from the scattering equation and we begin with this because it is simpler than the derivation of the full Fokker-Planck equation.

**The rescaling.** To achieve this goal, we assume that scattering occurs with small changes and a fast rate

$$\begin{cases}\frac{\partial}{\partial t}n_\varepsilon(t,x)+\frac{1}{\varepsilon}\left[k(x)n_\varepsilon(t,x)-\int_{\mathbb{R}^d}\frac{1}{\varepsilon^d}K(y,\frac{x-y}{\varepsilon})n_\varepsilon(t,y)dy\right]=0,\\ \\ n_\varepsilon(t=0,x)=n^0(x)\geq 0,\qquad \int_{\mathbb{R}^d}n^0(x)dx:=M^0.\end{cases}\tag{9.7}$$

Additionally to (9.2), we define and assume

$$U(x):=\int_{\mathbb{R}^d}zK(x,z)dz\in L^\infty(\mathbb{R}^d),\qquad \sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d}|z|^2K(x,z)dz<\infty,\tag{9.8}$$

$$\int_{\mathbb{R}^d}[K(y+\varepsilon z,z)-K(y,z)]dz\leq\varepsilon K_1.\tag{9.9}$$

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 $n_\varepsilon$ a subsequence such that for all $T>0$,

$$n_\varepsilon\rightharpoonup n\qquad\text{weakly in measures on } [0,T]\times\mathbb{R}^d.$$

it means that for $\Phi \in C_0\big((0,T)\times \mathbb{R}^d\big)$,

$$\int_0^T \int_{\mathbb{R}^d} n_\varepsilon(t,x)\Phi(t,x)dx\, dt \underset{\varepsilon\to 0}{\longrightarrow} \int_0^T \int_{\mathbb{R}^d} n(t,x)\Phi(t,x)dx\, dt.$$

This handles a very weak type of solutions.

We can prefer another route based on Relative Entropy, section 9.2 and assume that for a function $\overline{N} \in L^1\cap L^\infty(\mathbb{R}^d)$, the steady states $N_\varepsilon$ in (9.6) undergo the uniform control

$$0 \le n_\varepsilon^0 \le C_0 N_\varepsilon \le \overline{N}.$$

Then we may extract a subsequence such that

$$n_\varepsilon \rightharpoonup n \le \overline{N} \qquad \text{in } \; L^\infty(\mathbb{R}^+\times\mathbb{R}^d) - w* . \tag{9.10}$$

it 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 is rather restricitve although an example is built in section 9.5. That is the reason we derive a more general $L^2$ bound

**Uniform a priori estimate.**

**Lemma 9.4** *Assume* (9.2)*,* (9.9) *and that for some constant* $C_0$

$$\|n_\varepsilon^0\|_{L^2(\mathbb{R}^d)} \le C_0.$$

*Then for all times* $t \ge 0$ *we have*

$$\|n_\varepsilon(t)\|_{L^2(\mathbb{R}^d)} \le C_0 e^{K_1 t/2}.$$

**Proof**. We compute

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2dx + \frac{1}{\varepsilon}\int_{\mathbb{R}^d} k(x)n_\varepsilon(t,x)^2dx \; &= \frac{1}{\varepsilon^{d+1}}\int_{\mathbb{R}^d} K(y,\tfrac{x-y}{\varepsilon})n_\varepsilon(t,y)n_\varepsilon(t,x)dydx \\ &\le \frac{1}{2\varepsilon^{d+1}}\int_{\mathbb{R}^d} K(y,\tfrac{x-y}{\varepsilon})[n_\varepsilon(t,y)^2 + n_\varepsilon(t,x)^2]dydx.\end{aligned}$$

Using (9.2) and the change of variable $x \mapsto z = \frac{x-y}{\varepsilon}$, this reduces to

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2dx + \frac{1}{\varepsilon}\int_{\mathbb{R}^d} k(x)n_\varepsilon(t,x)^2dx \; &\le \frac{1}{\varepsilon}\int_{\mathbb{R}^d} K(y,z)n_\varepsilon(t,y-\varepsilon z)^2dydz \\ &\le \frac{1}{\varepsilon}\int_{\mathbb{R}^d} K(y'+\varepsilon z,z)n_\varepsilon(t,y')^2dy'dz.\end{aligned}$$

Using (9.2) again, this is also written

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx &\le \frac{1}{\varepsilon}\int_{\mathbb{R}^d}[K(y+\varepsilon z,z)-K(y,z)]n_\varepsilon(t,y)^2 dydz \\ &\le K_1\int_{\mathbb{R}^d} n_\varepsilon(t,y)^2 dy.\end{aligned}$$

The Gronwall lemma gives the conclusion. □

**The hyperbolic limit.** With this Lemma we can extract from $n_\varepsilon$ 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 9.5 (Hyperbolic limit for the scattering equation)** *Assume* (9.2)*,* (9.8)*,* (9.9) *and* $\|n_\varepsilon^0\|_{L^2(\mathbb{R}^d)} \le C_0$*. After extraction, the weak limit* $n$ *of the solution to* (9.7) *satisfies, in the distributional sense, the transport equation*

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) + \operatorname{div}\big(n(t,x)U(t,x)\big) = 0, \qquad t\ge 0,\ x\in\mathbb{R}^d, \\ n(t=0,x) = n^0(x). \end{cases} \tag{9.11}$$

**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 $t\ge T$ 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,

$$\begin{aligned}-\int_0^T\int_{\mathbb{R}^d}\frac{\partial}{\partial t}\Phi(t,x) \quad & n_\varepsilon(t,x) - \int_{\mathbb{R}^d}\Phi(0,x)n^0(x)dx \\ &= -\int_0^T\int_{\mathbb{R}^d} n_\varepsilon(t,x)\int K(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon}dz\, dx \\ &= -\int_0^T\int_{|z|\le R} n_\varepsilon(t,x)\int K(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon}dz\, dx + I_\varepsilon^R.\end{aligned}$$

It remains to handle these two terms. From the one hand

$$I_\varepsilon^R = \int_{|z|\le R} K(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon}dz,$$

and we can bound it using the second moment in (9.8)

$$\begin{aligned}|I_\varepsilon^R| &\leq \int_0^T \left[\int_{\mathbb{R}^d} n_\varepsilon(t,x)dx \ \sup_{x\in\mathbb{R}^d} \int_{|z|\geq R} K(x,z)\frac{|\Phi(t,x)-\Phi(t,x+\varepsilon z)|}{\varepsilon}dz\right] dt \\ &\leq T\ M^0 \|\nabla\Phi\|_\infty \ \sup_{x\in\mathbb{R}^d} \int_{|z|\geq R} K(x,z)|z|dz \\ &\leq \frac{T\ M^0}{R}\ \|\nabla\Phi\|_\infty \int_{|z|\geq R} K(x,z)|z|^2 dz \\ &\leq \frac{C}{R}\end{aligned}$$

for a constant $C$ independent of $\varepsilon$.

On the other hand, strongly in $L^2\big((0,T)\times\mathbb{R}^d\big)$,

$$\int_{|z|\leq R} K(x,z)\frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon}dz \underset{\varepsilon\to 0}{\longrightarrow} \int_{|z|\leq R} K(x,z)z.\nabla\Phi(t,x)dz \underset{R\to\infty}{\longrightarrow} U(x).\nabla\Phi(t,x). \tag{9.12}$$

Then by weak-strong convergence we find

$$-\int_0^T \int_{\mathbb{R}^d} \frac{\partial}{\partial t}\Phi(t,x)n(t,x) - \int_{\mathbb{R}^d} \Phi(0,x)n^0(x)dx = -\int_0^T \int_{\mathbb{R}^d} n(t,x)U(x).\nabla\Phi(t,x)dx.$$

This is the weak formulation of equation (9.11). □

## 9.4 The diffusive limit of scattering

The same ideas are involved to derive the Fokker-Planck equation from the scattering equations with a two scale limit this time.

### The rescaling

The Fokker-Planck equation can be derived from the scattering equation with a strong and balanced scale.

$$\frac{\partial}{\partial t}n_\varepsilon(t,x) + \frac{1}{\varepsilon^2}\left[k(x)n_\varepsilon(t,x) - \int_{\mathbb{R}^d} \frac{1}{\varepsilon^d}K_\varepsilon(y,\frac{x-y}{\varepsilon})n_\varepsilon(t,y)dy\right] = 0, \tag{9.13}$$

still with an initial data $n^0 \in L^1(\mathbb{R}^d)$. The kernel $K_\varepsilon$ depends only slightly on $\varepsilon$; we have in mind here a small asymmetry. Precisely, we make the assumptions,

$$K_\varepsilon(y,z) \geq 0, \qquad k(y) := \int_{\mathbb{R}^d} K_\varepsilon(y,z)dz \in L^\infty(\mathbb{R}^d), \tag{9.14}$$

$$\int_{\mathbb{R}^d} (1+|z|^3)K_\varepsilon(y,z)dz \in L^\infty(\mathbb{R}^d), \tag{9.15}$$

$$\int_{\mathbb{R}^d} zK_\varepsilon(y,z)dz = \varepsilon U(y), \qquad \int_{\mathbb{R}^d} z_i z_j K_\varepsilon(y,z)dz = A_{ij}(y), \tag{9.16}$$

$$U_i,\ A_{ij} \in C \cap L^\infty(\mathbb{R}^d), \qquad (A_{ij}) \text{ is a definite positive matrix,} \tag{9.17}$$

(here $i,\ j = 1, ..., I$). Notice that $A_{ij}(x)$ is a symmetric matrix by its construction.

**Theorem 9.6** *After extraction, in the sense of* (9.10)*, the weak limit $n$ of the solution $n_\varepsilon$ to* (9.13) *satisfies in the distributional sense*

$$\frac{\partial}{\partial t} n(t,x) - \frac{1}{2}\sum_{i,j=1}^{I} \frac{\partial^2}{\partial_{x_i}\partial_{x_j}}\big[A_{ij}(x)n(t,x)\big] + \operatorname{div}\big[U(x)n(t,x)\big] = 0,$$

*with the initial data $n^0$.*

**Proof**. We change variables from $y$ to $z = \frac{x-y}{\varepsilon}$ and arrive to the formulation

$$\frac{\partial}{\partial t} n_\varepsilon(t,x) + \int \frac{1}{\varepsilon^2}\big[K_\varepsilon(x,z)n_\varepsilon(t,x) - K_\varepsilon(x-\varepsilon z, z)n_\varepsilon(t, x-\varepsilon z)\big]dz = 0.$$

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 we can write

$$\begin{aligned}\int\int n_\varepsilon(t,x)K_\varepsilon(x,z) & \ \frac{\Phi(t,x)-\Phi(t,x+\varepsilon z)}{\varepsilon^2}dz\ dx \\ &= \int\int n_\varepsilon(t,x)K_\varepsilon(x,z)\left[-\frac{z.\nabla\Phi(t,x)}{\varepsilon} - \frac{z_i z_j}{2}D^2_{ij}\Phi(t,x)\right]dz\ dx + O(\varepsilon).\end{aligned}$$

And thus, we arrive at

$$\begin{aligned}-\int \tfrac{\partial}{\partial t}\Phi(t,x)n_\varepsilon(t,x) + \int n_\varepsilon(t,x) & \ \left[-U(x).\nabla\Phi(t,x)\big((0,T)\times\mathbb{R}^d\big)\big) - \tfrac{1}{2}A_{ij}(x)D^2_{ij}\Phi(t,x)\right]dx \\ &= \int \Phi(0,x)n^0(x)dx + O(\varepsilon).\end{aligned}$$

We may pass to the limit and obtain the result. $\square$

## 9.5 Construction of the integral kernel

One can also address the reverse question: being given the coefficients $U(\cdot) \in L^\infty(\mathbb{R}^d)^d$ and $A(\cdot) \in L^\infty(\mathbb{R}^d)^{d\times d}$, a definite positive symmetric matrix, can one build an appropriate kernel $K_\varepsilon$ that gives the moments in (9.15), (9.16). To do so, it is enough to choose $k(y) \equiv 1$ and to use the formula

$$K_\varepsilon(y,z) = \det A^{-1/2}\ \mathcal{K}\left(\left|A(y)^{-1/2}.(z-\varepsilon U(y))\right|^2\right),$$

with $A(y)^{-1/2}$ the unique definite positive symmetric matrix such that $A(y)^{-1/2}.A(y)^{-1/2} = A(y)^{-1}$ and $\mathcal{K} : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ 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 instance a normalized gaussian will do it.

Indeed, after the change of variable $z \mapsto \eta = A(y)^{-1/2}.(z - \varepsilon U(y))$, $d\eta = \det A^{-1/2}(y)\, dz$, 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,

$$\int_{\mathbb{R}^d} (z - \varepsilon U(y))K_\varepsilon(y,z)dz = \int_{\mathbb{R}^d} A(y)^{1/2}.\eta\mathcal{K}\left(|\eta|^2\right) d\eta = 0.$$

Finally, we also compute using the previous relations

$$\begin{aligned} \textstyle\int_{\mathbb{R}^d} z_i z_j K_\varepsilon(y,z)dz &= \textstyle\int_{\mathbb{R}^d} (z_i - \varepsilon U_i(y))(z_j - \varepsilon U_j(y))K_\varepsilon(y,z)dz - \varepsilon^2 U_i(y)U_j(y) \\ &= \textstyle\int_{\mathbb{R}^d} (A(y)^{1/2}.\eta)_i.(A(y)^{1/2}.\eta)_j\ \mathcal{K}\left(|\eta|^2\right) d\eta - \varepsilon^2 U_i(y)U_j(y) \\ &= A_{ij}(y) - \varepsilon^2 U_i(y)U_j(y) \end{aligned}$$

because

$$\begin{aligned} \textstyle\int_{\mathbb{R}^d} (A(y)^{1/2}.\eta)_i.(A(y)^{1/2}.\eta)_j\ \mathcal{K}\left(|\eta|^2\right) d\eta &= \textstyle\sum_{k,l} \int_{\mathbb{R}^d} (A(y)^{1/2}_{ik}.\eta_k\ A(y)^{1/2}_{lj}.\eta_l\ \mathcal{K}\left(|\eta|^2\right) d\eta \\ &= \textstyle\sum_k (A(y)^{1/2}_{ik}\ A(y)^{1/2}_{kj} = A_{ij}(y). \end{aligned}$$

This is not exactly the second relation (9.16) because of the term $-\varepsilon^2 U_i(y)U_j(y)$. This is not a real difficulty, we can either change $A_{ij}$ in our construction and replace it by $A_{ij} + \varepsilon^2 U_i(y)U_j(y)$, either notice that a correction in $\varepsilon^2$ does not change the limit in Theorem 9.6.

### Further a priori estimates on $n_\varepsilon$

With little more assumptions, the weak limit in (**??**) can be made stronger. To do so we assume a second order expansion of $K_\varepsilon$ along with (9.16),

$$\left(\int_{\mathbb{R}^d} K_\varepsilon(x - \varepsilon z, z)dz - k(x)\right)_+ \leq L_2\varepsilon^2, \tag{9.18}$$

which implies that

$$\left(-\mathrm{divU} + \frac{1}{2}\sum_{i,j} D^2_{ij}A_{ij}\right)_+ \in L^\infty(\mathbb{R}^d).$$

**Proposition 9.7** *With the assumption* (9.18), *we have*

$$\|n_\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \leq \|n^0(\cdot)\|_{L^2(\mathbb{R}^d)} e^{2L_2 t}.$$

**Proof**. We compute

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^{2d}} K(x-\varepsilon z, z) n_\varepsilon(t, x-\varepsilon z) n_\varepsilon(t,x) dz\, dx - \int_{\mathbb{R}^d} k(x) n_\varepsilon(t,x)^2 dx\right].$$

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 (9.14),

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx = \frac{1}{\varepsilon^2}\left[\int_{\mathbb{R}^{2d}} K(x-\varepsilon z, z) n_\varepsilon(t,x)^2 dz\, dx - \int_{\mathbb{R}^d} k(x) n_\varepsilon(t,x)^2 dx\right].$$

Now, using (9.18), we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx = L_2 \int_{\mathbb{R}^d} n_\varepsilon(t,x)^2 dx,$$

and the result follows. $\square$

# Chapter 10

# Dynamical patterns

So far we have shown, using the concept of Turing Instability, that patterns can occur as steady states and many examples. Other patterns can grow with time, thus generating dynamical patterns. We give several examples now.

## 10.1 Unstable traveling waves: the diffusive Fisher equation

## 10.2 Gray-Scott system (2)

We consider the particular case $n = 2$, $B = 0$ in the Gray-Scott system (7.22), which is then written as

$$\begin{cases} \dfrac{\partial u}{\partial t} - d_u \Delta u = u^2 v - Au, \\ \dfrac{\partial v}{\partial t} - d_v \Delta v = -u^2 v. \end{cases} \tag{10.1}$$

It is already very rich and exhibits beautiful dynamical patterns shown in Figures 10.1 and 10.2. These are not Turing patterns because there is no unstable steady state in this particular case. In fact the only steady state is obviously $(0, 0)$ which is stable.

## 10.3 Mimura system for dentritic bacterial colonies

Bacterial colonies often exhibit remarkable patterns, see Figure 10.4 for instance. They follow from complex collective interactions between cells due to several effects: random motion of the individual cells, cell division and colony growth, release of various molecules in their environment resulting e.g. in chemoattraction or surface tension (see [26]). The patterns depend heavily on the type of bacteria and on the support used for the experiment (solid, semi-solid, liquid). A

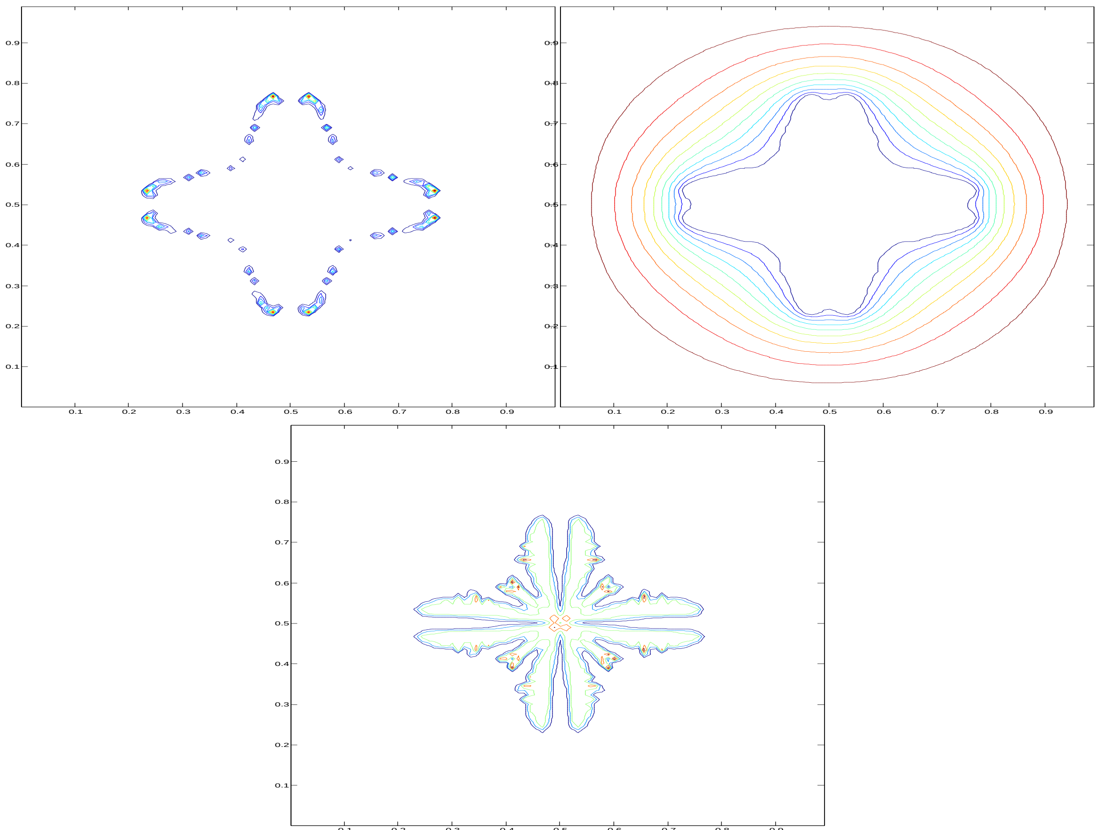

Figure 10.1: Two dimensional simulations of the Gray-Scott system (10.1) on a square grid (the quantities $u$, $v$ and $\int_0^t u(x,s)ds$ are depicted).

good account on this issue can be found in Murray's book [41].

A simple model for dentritic colonies growth is due to Mimura [39]. It takes into account only three simple effects: (i) a brownian motion of actives cells which density is denoted by $n(t,x)$ below, (ii) a nutrient of concentration $c(t,x)$ which is diffused in the medium an 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 (10.2) and numerical results are presented in Figures 10.5 and 10.6. It is well established that the biophysical ingredients of this model are not those in the real experiments leading to Figure 10.4, nevertheless they share several common patterns.

$$\begin{cases} \frac{\partial}{\partial t} n(t,x) - d_1 \Delta n(t,x) = n \left( c - \frac{1}{(1+n)\,(1+c)} \right), \quad t \geq 0,\ x \in \mathbb{R}^2, \\ \frac{\partial}{\partial t} c(t,x) - d_2 \Delta c(t,x) = -nc, \\ \frac{\partial}{\partial t} f(t,x) = n\, \frac{1}{(1+n)\,(1+c)}. \end{cases} \tag{10.2}$$

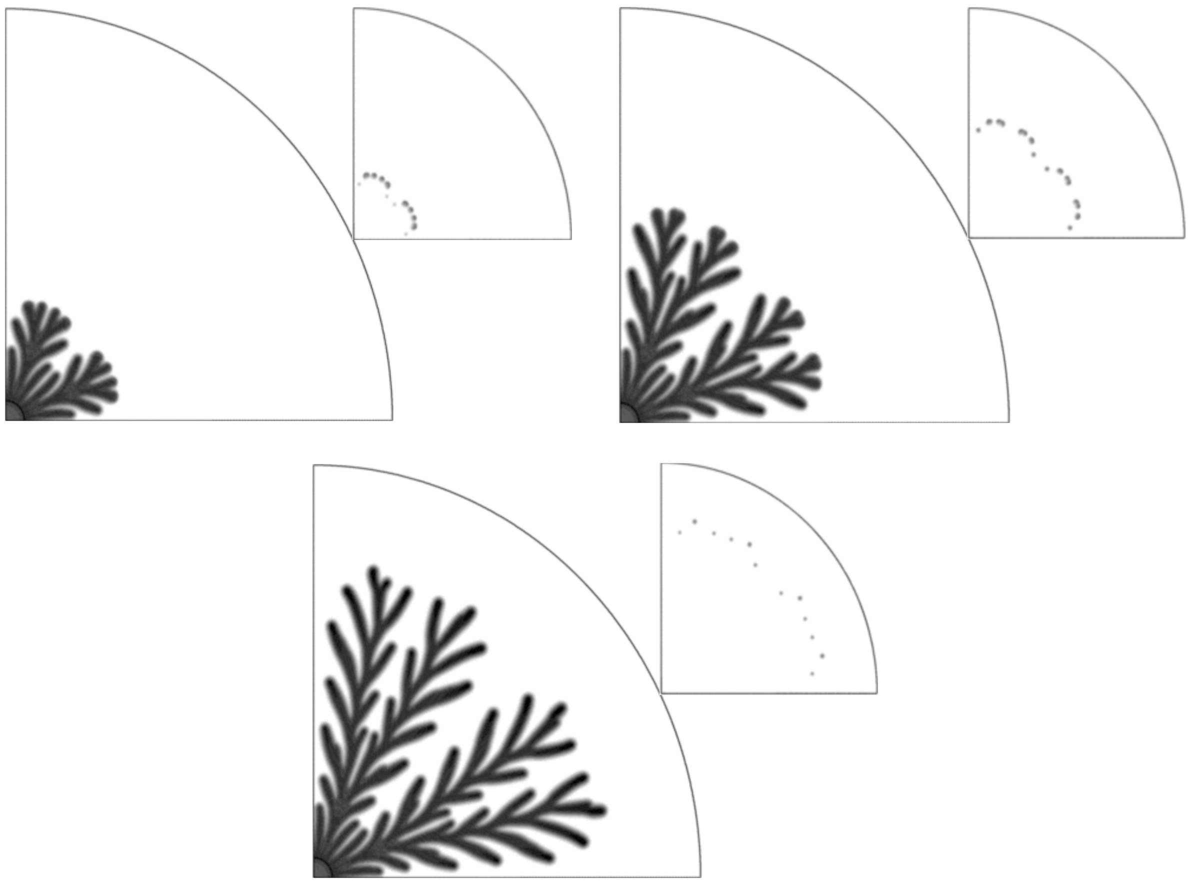

Figure 10.2: Simulations of the Gray-Scott system (10.1) on an unstructured grid: the quantities $\int_0^t u(x,s)ds$ (large quadrant) and $u(x,t)$ (small quadrant). The solutions at three different times are shown. Computations by A. Marrocco.

The initial data represents an *inoculum*, i.e., a large amount of bacteria located at the center of the ball (the computational domain). The reason why the dentritic pattern occurs in this model is that the solution $n(t,x)$ to the first equation has a tendency to create Dirac concentrations. These concentrations move towards the larger values of the nutrient $c$, and this is the boundary of the computational domain. Indeed, the nutrient is consumed progressively inside the domain and this creates a nutrient gradient towards the exterior.

## 10.4 Spiral waves

Spiral waves are observed in various fields of sciences. Two typical examples are the Belousov-Zabotinsky chemical reaction and electrophysiology where they are responsible of fibrillation.

Parabolic systems such as the FitzHugh-Nagumo in two dimensions are able to produce this

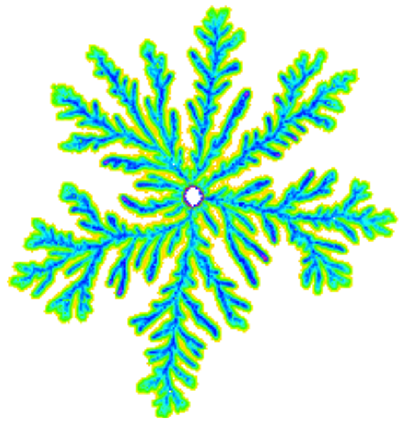

Figure 10.3: Another simulations of the Gray-Scott system (10.1) on an unstructured grid: the quantities $\int_0^t u(x,s)ds$. Computations by S. M. Kaber based on FreeFem++.

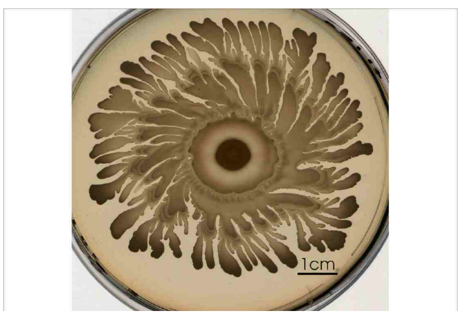



Figure 10.4: BACTERIAL COLONIES OF SALMONELLA *Bacillus Subtilis*. EXPERIMENTS BY S. SEROR *et al*, INSTITUT DE GÉNÉTIQUE ET MICROBIOLOGIE, UNIVERSITÉ PARIS-SUD.

type of solutions in a range of parameters where the constant steady state is Turing unstable (see section 7.6.7). We use the system is written

$$\begin{cases} \tau \frac{\partial}{\partial t} u(t,x) - d\Delta u(t,x) &= u - \frac{u^3}{3} - v, \quad t \geq 0, \ x \in [0,1]^2, \\ \frac{\partial}{\partial t} c(t,x) &= -u - c - \gamma v. \end{cases} \tag{10.3}$$

Numerical solutions are obtained with an initial data displayed in Figure 10.7.

## 10.5 Liesegang rings

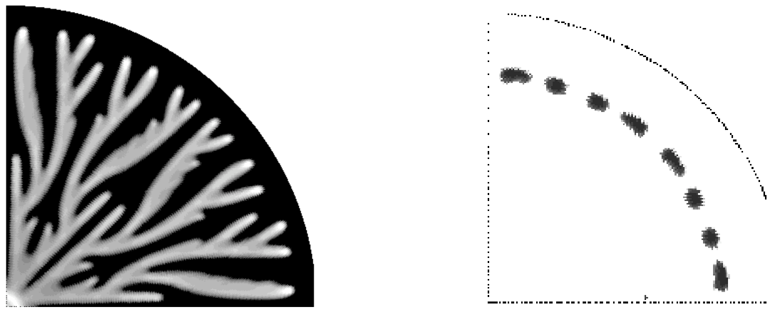

Figure 10.5: Solutions of Mimura's system (10.2) at a fixed time.Left: frozen bacteria $f(t,x)$. Right: active bacteria $n(t,x)$. Computations by A. Marrocco.

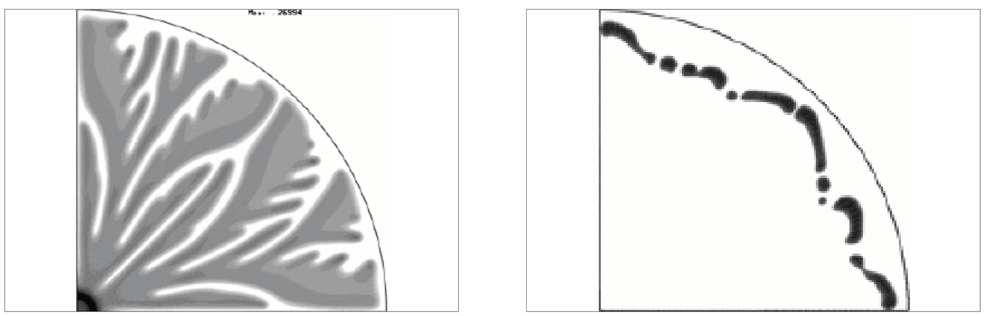

Figure 10.6: Solutions of Mimura's system (10.2) with a higher nutrient level $S$ than in Figure 10.5. Computations by A. Marrocco.

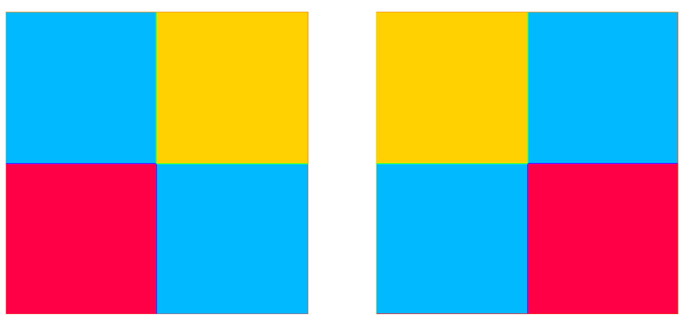

Figure 10.7: Initial data in system (10.3). Red=1, Blue=0, yellow=-1 and represent the three steady states of the system.

Figure 10.8: Snapshot of the solution to system (10.3) at three different times for parameters $\tau = 0.01$, $c = 0.2$, $d = 10^{-5}$, $\gamma = 0.5$.

# Chapter 11

# Strong reactions and the Stefan free boundary problem

Departing from reaction-diffusion systems one can rescale the problem and consider the global length of the (experimental, computational, observation) domain rather the natural scale which, e.g. in population biology, is the individual size scale. Doing so we rescale the space variable and this leads to also rescale time so as to use the propagation time scale rather the generation scale.

There are many different ways to change scale and we will discuss several of them in the next chapters.

Here we give the example of the *hyperbolic scale* where the old time is defined as $\widetilde{t} = \frac{t}{\varepsilon}$, with $t$ the new time. Then we also replace the old space variable $\widetilde{x}$ by $x$ with the relation $\widetilde{x} = \frac{x}{\sqrt{\varepsilon}}$ so as to keep the velocity ratio $x/t$ unchanged..

## 11.1 Derivation of the Stefan problem (no latent heat)

As a first and simple example, consider the reaction-diffusion equation

$$\begin{cases} \frac{\partial}{\partial t} u_\varepsilon - d_1 \Delta u_\varepsilon = -\frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} v_\varepsilon - d_2 \Delta v_\varepsilon = -\frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \\ u_\varepsilon(t=0,x) = u^0_\varepsilon(x) \geq 0, \qquad v_\varepsilon(t=0,x) = v^0(x) \geq 0, \qquad u^0_\varepsilon,\ v^0_\varepsilon \in L^\infty \cap L^1(\mathbb{R}^d) \ \text{(uniformly in } \varepsilon). \end{cases} \tag{11.1}$$

Because the right hand sides are nonpositive, it is easy to see that there is a unique solution and that for all $t \geq 0$

$$0 \leq u_\varepsilon(t,x) \leq \|u^0_\varepsilon\|_\infty, \qquad 0 \leq v_\varepsilon(t,x) \leq \|v^0_\varepsilon\|_\infty, \tag{11.2}$$

$$
\begin{cases} \displaystyle\int_{\mathbb{R}^d} u_\varepsilon(t,x)dx + \int_0^t \int_{\mathbb{R}^d} \frac{u_\varepsilon(s,x)v_\varepsilon(s,x)}{\varepsilon} dxds \le \int_{\mathbb{R}^d} u_\varepsilon^0(x)dx, \\ \displaystyle\int_{\mathbb{R}^d} v_\varepsilon(t,x)dx + \int_0^t \int_{\mathbb{R}^d} \frac{u_\varepsilon(s,x)v_\varepsilon(s,x)}{\varepsilon} dxds \le \int_{\mathbb{R}^d} v_\varepsilon^0(x)dx. \end{cases} \tag{11.3}
$$

This is already a significant piece of information because it tells us that $u_\varepsilon v_\varepsilon$ should vanish as $\varepsilon$ tends to 0.

We can also obtain stronger a priori estimates under the $TV$ assumption

$$
\|\nabla u_\varepsilon^0\|_1 + \|\nabla v_\varepsilon^0\|_1 \le C^0, \tag{11.4}
$$

and for well prepared initial data

$$
\left\| d_1 \Delta u_\varepsilon^0 - \frac{u_\varepsilon^0 v_\varepsilon^0}{\varepsilon} \right\|_1 + \left\| d_2 \Delta v_\varepsilon^0 - \frac{u_\varepsilon^0 v_\varepsilon^0}{\varepsilon} \right\|_1 \le C^1. \tag{11.5}
$$

Then, we obtain the

**Theorem 11.1** *Consider equation (11.1) with assumptions* (11.4)–(11.5)*. Then, additionally to the a priori bounds* (11.2) *and* (11.3)*, we have for all* $t \ge 0$*,*

$$
\|\nabla u_\varepsilon(t)\|_1 + \|\nabla v_\varepsilon(t)\|_1 \le \|\nabla u_\varepsilon^0\|_1 + \|\nabla v_\varepsilon^0\|_1 := C^0,
$$

$$
\|\frac{\partial u_\varepsilon(t)}{\partial t}\|_1 + \|\frac{\partial v_\varepsilon(t)}{\partial t}\|_1 \le C^1.
$$

$$
u_\varepsilon \to u, \qquad v_\varepsilon \to v \qquad \textit{strongly in } \; L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^d),
$$

$$
u,\, v \in L^\infty\big(\mathbb{R}^+; L^1 \cap L^\infty(\mathbb{R}^d)\big), \qquad u(t,x)\; v(t,x) = 0 \; a.e.
$$

*and* $w = u - v$ *satisfies the Stefan problem (11.6),* (11.7) *below.*

**Remark 11.2** *One can avoid the assumption taht the initial data is well-prepared* (11.5)*. Then time compactness comes from Lions-Aubin lemma, see Appendix 13.1 One just uses from the proof below that*

$$
\frac{\partial}{\partial t} u_\varepsilon = \Delta(d_1 u_\varepsilon) + r_\varepsilon(t,x), \qquad \frac{\partial}{\partial t} v_\varepsilon = \Delta(d_2 v_\varepsilon) + r_\varepsilon(t,x),
$$

*with* $(d_1 u_\varepsilon)$ *and* $(d_2 v_\varepsilon)$ *compact in space and* $r_\varepsilon$ *bounded in* $L^1_{t,x}$*. In these conditions compactness in time follows.*

**Proof**.

*First step. Derivation of the Stefan problem.* We fist show why the singular limit of (11.1) is described by the Stefan problem without latent heat

$$
\frac{\partial}{\partial t} w - \Delta A(w) = 0, \qquad t \ge 0,\; x \in \mathbb{R}^d, \tag{11.6}
$$

with

$$A(w) = \begin{cases} d_2 w & \text{for } w \leq 0, \\ d_1 w & \text{for } w \geq 0. \end{cases} \tag{11.7}$$

Figure 11.1 shows this finction $A(\cdot)$ together with the case with latent heat for comparison.

The derivation is as follows. With the $TV$ estimates stated in Theorem 11.1, the families $u_\varepsilon$ and $v_\varepsilon$ are locally compact in $L^1_{t,x}$ and we may extract subsequences, that we still denote $u_\varepsilon$ and $v_\varepsilon$, that converge almost everywhere. From the estimate on $u_\varepsilon v_\varepsilon$ stated in (11.3), we deduce

$$u\, v = \lim_{\varepsilon \to 0} u_\varepsilon v_\varepsilon = 0. \tag{11.8}$$

Next, we define

$$w_\varepsilon = u_\varepsilon - v_\varepsilon \underset{\varepsilon \to 0}{\longrightarrow} w = u - v.$$

We write, substracting the equations on $u_\varepsilon$ and $v_\varepsilon$,

$$\frac{\partial}{\partial t} w_\varepsilon - \Delta[d_1 u_\varepsilon - d_2 v_\varepsilon] = 0.$$

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 $u(t,x) > 0$, therefore $v_\varepsilon(t,x) \to v(t,x) = 0$ 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 $v(t,x) < 0$, therefore $u_\varepsilon(t,x) \to u(t,x) = 0$ 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 $u_\varepsilon$ and $v_\varepsilon$. 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 to (11.6), and thus of the limit (a fact that we do not prove here, see [15]).

We now prove the $TV$ estmates in $x$. We work on the equations of (11.1) and differentiate them with respect to $x_i$. We multiply by the sign and obtain

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{R}^d} \quad & \Big[|\tfrac{\partial}{\partial x_i} u_\varepsilon(t,x)| + |\tfrac{\partial}{\partial x_i} v_\varepsilon(t,x)|\Big]\, dx \\ & \leq -\int_{\mathbb{R}^d} [\tfrac{\partial}{\partial x_i} u_\varepsilon\ v_\varepsilon + u_\varepsilon\ \tfrac{\partial}{\partial x_i} v_\varepsilon] \Big[\mathrm{sgn}\big(\tfrac{\partial}{\partial x_i} u_\varepsilon(t,x)\big) + \mathrm{sgn}\big(\tfrac{\partial}{\partial x_i} v_\varepsilon(t,x)\big)\Big] \\ & = -\int_{\mathbb{R}^d} \Big[|\tfrac{\partial}{\partial x_i} u_\varepsilon(t,x)| v_\varepsilon + |\tfrac{\partial}{\partial x_i} v_\varepsilon(t,x)| u_\varepsilon + \tfrac{\partial}{\partial x_i} u_\varepsilon(t,x) \mathrm{sgn}\big(\tfrac{\partial}{\partial x_i} v_\varepsilon\big) v_\varepsilon + \tfrac{\partial}{\partial x_i} v_\varepsilon(t,x) \mathrm{sgn}\big(\tfrac{\partial}{\partial x_i} u_\varepsilon(t,x)\big) u_\varepsilon\Big] \\ & \leq 0.\end{aligned}$$

this is exactly the first estimate stated in Theorem 11.1.

*Third step. Derivation of the $TV$ estimate in $t$.*

the same calculation as before 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 $t = 0$,

$$\begin{aligned}\|\tfrac{\partial}{\partial t} u_\varepsilon(t)\|_1 + \|\tfrac{\partial}{\partial t} v_\varepsilon(t)\|_1 \quad & \leq \|\tfrac{\partial}{\partial t} u^0_\varepsilon\|_1 + \|\tfrac{\partial}{\partial t} v^0_\varepsilon\|_1 \\ & = \Big\| d_1 \Delta u^0_\varepsilon - \tfrac{u^0_\varepsilon v^0_\varepsilon}{\varepsilon}\Big\|_1 + \Big\| d_2 \Delta v^0_\varepsilon - \tfrac{u^0_\varepsilon v^0_\varepsilon}{\varepsilon}\Big\|_1 \quad .\end{aligned}$$

This proves the second estimate stated in Theorem 11.1 and concludes its proof. □

## 11.2 Stefan problem with reaction terms

An extension of the Stefan problem without latent heat can be obtained included reaction terms[1] and the simplest example is

$$\begin{cases} \frac{\partial}{\partial t} u_\varepsilon - d_1 \Delta u_\varepsilon = f(u_\varepsilon) - \frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \qquad t \geq 0,\ x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t} v_\varepsilon - d_2 \Delta v_\varepsilon = g(u_\varepsilon) - \frac{1}{\varepsilon} u_\varepsilon v_\varepsilon, \\ u_\varepsilon(t=0,x) = u^0(x) \geq 0, \qquad v_\varepsilon(t=0,x) = v^0(x) \geq 0, \qquad u^0,\ v^0 \in L^\infty \cap L^1(\mathbb{R}^d). \end{cases} \tag{11.9}$$

In ecology this represents two species that follow, in the absence of the other species, two independent Fisher equations and then we obtain the reaction terms

$$f(u) = r_1 u(c_1 - u), \qquad g(u) = r_2 u(c_2 - u).$$

[1]The stationary problem in a bounded domain was studied by E. N. Dancer and Y. Du, Competing species equations with diffusion, large interactions and jumping singularities, Journal of Differential Equations, 114 (1994), 434–475.

Additionally these species undergo a very strong competition.

The singular limit of (11.1) is described by the Stefan problem without latent heat

$$\frac{\partial}{\partial t}w - \Delta A(w) = f(w_+) - g(w_-), \qquad t \geq 0,\ x \in \mathbb{R}^d, \tag{11.10}$$

still with the definitions $w = \lim_{\varepsilon\to 0}(u_\varepsilon - v_\varepsilon)$ and $A(\cdot)$

$$A(w) = \begin{cases} d_2 w & \text{for } w \leq 0, \\ d_1 w & \text{for } w \geq 0. \end{cases}$$

The derivation of this system follows exactly the same steps as the simpler case treated in Section 11.2.

## 11.3 Derivation of the Stefan problem with latent heat

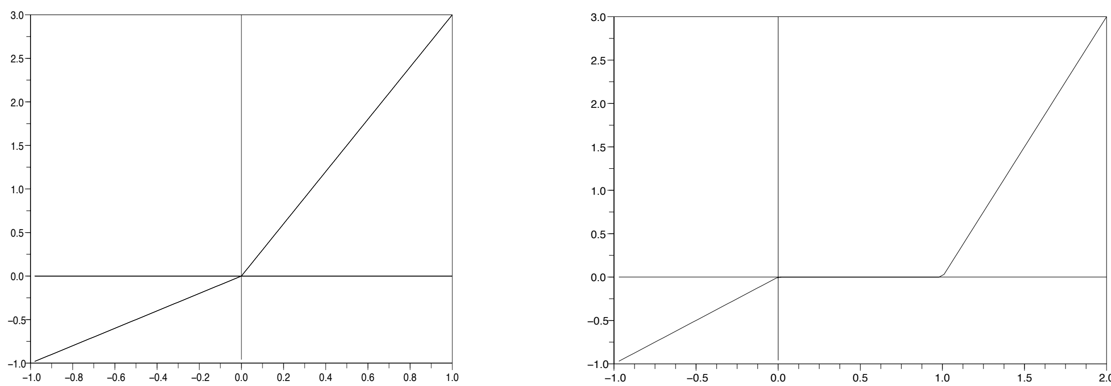


Figure 11.1: The nonlinear diffusions in Stefan problems. Left: no latent heat, the function $A(\cdot)$ according to (11.6),(11.7). Left: with latent heat $\lambda = 1$ here, the function $B(\cdot)$ according to (11.12),(11.13).

In order to include latent heat in the Stefan problem, the reaction-diffusion system (11.1) can be extended with a third equation. Following [28], we consider the semilinear system

$$\begin{cases} \frac{\partial}{\partial t}u_\varepsilon - d_1\Delta u_\varepsilon = -\frac{1}{\varepsilon}u_\varepsilon\big[v_\varepsilon + \lambda(1-p_\varepsilon)\big], & t \geq 0,\ x \in \mathbb{R}^d, \\ \frac{\partial}{\partial t}v_\varepsilon - d_2\Delta v_\varepsilon = -\frac{1}{\varepsilon}v_\varepsilon(u_\varepsilon + \lambda p_\varepsilon), \\ \frac{\partial}{\partial t}p_\varepsilon = \frac{1}{\varepsilon}\big[(1-p_\varepsilon)u_\varepsilon - v_\varepsilon p_\varepsilon\big], \end{cases} \tag{11.11}$$

and we give initital data satisfying (with uniform upper bounds in $\varepsilon$)

$$0 \leq u^0_\varepsilon \leq \|u^0_\varepsilon\|_\infty, \qquad 0 \leq v^0_\varepsilon \leq \|v^0_\varepsilon\|_\infty, \qquad 0 \leq p^0_\varepsilon \leq 1.$$

The quantity $\lambda > 0$ is called the *latent heat*.

The invariant region for this system follows from the maximum principle

**Lemma 11.3** *There is a weak solution to* (11.11) *satisfying for all times*

$$u_\varepsilon(t) \geq 0, \qquad v_\varepsilon(t) \geq 0, \qquad 0 \leq p_\varepsilon(t) \leq 1.$$

**Proof**. The equations on $u_\varepsilon$ and $v_\varepsilon$ are Lotka-Volterra equations and the first two inequalities are just consequences of the general positivity principle in Lemma 1.1 and the construction method in Section 3.11.

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 $p_\varepsilon - 1 \leq 0$. □

We insist on the difference of scaling between the system at hand and that, formally close, in Section 11.2. This changes completely the asymptotic limit $\varepsilon \to 0$ that we study now.

We are going to derive the general Stefan problem with latent heat

$$\frac{\partial}{\partial t} w - \Delta B(w) = 0, \qquad t \geq 0,\ x \in \mathbb{R}^d, \tag{11.12}$$

with the definition of the diffusion nonlinearity $B(\cdot)$

$$B(w) = \begin{cases} d_2 w & \text{for } w \leq 0, \\ 0 & \text{for } 0 \leq w \leq \lambda, \\ d_1(w-1) & \text{for } w \geq \lambda. \end{cases} \tag{11.13}$$

See Figure 11.1.

The quantity $w$ is more complicated than in section 11.1 and 11.2. We define

$$w_\varepsilon = u_\varepsilon - v_\varepsilon + \lambda p_\varepsilon. \tag{11.14}$$

In the strong limits of $u_\varepsilon$, $v_\varepsilon$ and $p_\varepsilon$, 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 (11.11), that is

$$\begin{cases} u(t,x) > 0 \implies & v + \lambda(1-p) = 0 & \implies v = 0,\ p = 1, \\ v(t,x) > 0 \implies & u + \lambda p = 0 & \implies u = 0,\ p = 0, \\ & u(1-p) - vp = 0. & \end{cases}$$

The last line is a consequence of the first two limits. These two are enough to characterize our function $w$ defined above as

$$w = u - v + \lambda p = \begin{cases} -v & \text{for} \quad v > 0,\ u = 0,\ p = 0 \iff w < 0, \\ \in [0, \lambda] & \text{for} \quad v = 0,\ u = 0,\ p \geq 0 \iff w \in [0, \lambda], \\ \lambda + u & \text{for} \quad u > 0,\ v = 0,\ p = 1 \iff w > \lambda, \end{cases}$$

To conclude, we add up the equations of the system (11.11) (after pultiplying the second one by $-1$ and last one by $\lambda$), we find

$$\frac{\partial}{\partial t}[u_\varepsilon - v_\varepsilon + \lambda p_\varepsilon] - \Delta[d_1 u_\varepsilon - d_2 v_\varepsilon] = 0.$$

That 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 (11.13).

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 $u_\varepsilon$, $v_\varepsilon$ and $p_\varepsilon$. This comes under the additional $TV$ assumptions on the initial data

$$\|\nabla u_\varepsilon^0\|_1 + \|\nabla v_\varepsilon^0\|_1 + \|\nabla p_\varepsilon^0\|_1 \leq C^0, \tag{11.15}$$

and, for $TV$ estimates in time

$$\begin{cases} \big\| d_1 \Delta u_\varepsilon^0 - \frac{1}{\varepsilon} u_\varepsilon^0 \big[ v_\varepsilon^0 + \lambda(1 - p_\varepsilon^0 \big\| \leq C^1, \\ \big\| d_2 \Delta v_\varepsilon^0 - \frac{1}{\varepsilon} v_\varepsilon^0 (u_\varepsilon^0 + \lambda p_\varepsilon^0) \big\| \leq C^1, \\ \big\| \frac{\lambda}{\varepsilon} \big[ (1 - p_\varepsilon^0) u_\varepsilon^0 - v_\varepsilon^0 p_\varepsilon^0 \big\| \leq C^1. \end{cases} \tag{11.16}$$

We summarize our conclusions in the following statement

**Theorem 11.4** *Consider equation (11.11) with assumptions* (11.16)–(11.16). *Then, additionally to the a priori bounds in Lemma 11.3, we have for all $t \geq 0$,*

$$\|\nabla u_\varepsilon(t)\|_1 + \|\nabla v_\varepsilon(t)\|_1 + \lambda \|\nabla p_\varepsilon(t)\|_1 \leq \|\nabla u_\varepsilon^0\|_1 + \|\nabla v_\varepsilon^0\|_1 + \lambda \|\nabla_\varepsilon^0\|_1 := C^0,$$

$$\|\frac{\partial u_\varepsilon(t)}{\partial t}\|_1 + \|\frac{\partial v_\varepsilon(t)}{\partial t}\|_1 + \lambda \|\frac{\partial p_\varepsilon(t)}{\partial t}\|_1 \leq 3/; C^1.$$

$$u_\varepsilon \to u, \qquad v_\varepsilon \to v, \qquad p_\varepsilon \to p \qquad \textit{strongly in } \; L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^d),$$

$$u,\, v,\, p \in L^\infty\big(\mathbb{R}^+; L^1 \cap L^\infty(\mathbb{R}^d)\big),$$

$$u\,\big(v + \lambda(1-p)\big) = 0, \qquad v\,\big(u + \lambda p\big) = 0, \qquad u(1-p) - vp = 0,$$

*and $w = u - v + \lambda p$ satisfies the Stefan problem with latent heat $\lambda$ (11.12),* (11.13).

**Proof**. We only prove the $TV$ estimate in space; the other statements follow the same lines as in section 11.1. To simplify motations, we set $u_i = \frac{\partial u_\varepsilon}{\partial x_i}$. Once differentitated in $x_i$, the equations in (11.11) give

$$\begin{cases} \frac{\partial u_i}{\partial t} - d_1 \Delta u_i & = -\frac{u_i}{\varepsilon}\big(v + \lambda(1-p)\big) - \frac{u}{\varepsilon}\big(v_i - \lambda p_i\big), \\ \frac{\partial v_i}{\partial t} - d_2 \Delta v_i & = -\frac{v_i}{\varepsilon}\big(u + \lambda p\big) - \frac{v}{\varepsilon}\big(u_i + \lambda p_i\big), \\ \qquad\quad \frac{\partial p_i}{\partial t} & = -\frac{p_i}{\varepsilon}\big(u + v\big) + \frac{1}{\varepsilon}\big(u_i(1-p) - v_i p\big). \end{cases}$$

After multiplying each equation by the sign of the corresponding quantity according to Chapter 3, we find

$$\begin{cases} \frac{\partial |u_i|}{\partial t} - d_1 \Delta |u_i| & \leq -\frac{|u_i|}{\varepsilon}\big(v + \lambda(1-p)\big) + \frac{u}{\varepsilon}\big(|v_i| + \lambda |p_i|\big), \\ \frac{\partial |v_i|}{\partial t} - d_2 \Delta |v_i| & \leq -\frac{|v_i|}{\varepsilon}\big(u + \lambda p\big) + \frac{v}{\varepsilon}\big(|u_i| + \lambda |p_i|\big), \\ \qquad\quad \frac{\partial |p_i|}{\partial t} & \leq -\frac{|p_i|}{\varepsilon}\big(u + v\big) + \frac{1}{\varepsilon}\big(|u_i|(1-p) + |v_i| p\big). \end{cases}$$

Then, the combination $|u_i| + |v_i| + \lambda |p_i|$ makes that the terms of the right hand sides compensate and we find

$$\frac{\partial}{\partial t}\big[|u_i| + |v_i| + \lambda |p_i|\big] - \Delta[d_1|u_i| + d_2|v_i|] \leq 0.$$

We conclude that

$$\frac{d}{dt}\int_{\mathbb{R}^d} \big[|u_i| + |v_i| + \lambda|p_i|\big]dx \leq 0$$

and the $TV$ estimate of Theorem 11.4 follows. □

## 11.4 The geometric interpretation

The Stefan problem with latent heat admits a geometric interpretation; that means that one can also describe it by the velocity of the interface between the two phases.

The mushy region refers to the points where $0 \leq w(x,t) \leq \lambda$ in the Stefan problem (11.12),(11.13). In phase transitions, the set $\Omega_s(t) = \{x \text{ s.th. } w(x,t) < 0\}$ represents the solid state of the melting material. The set $\Omega_l(t) = \{x \text{ s.th. } w(x,t) > 0\}$ represents the liquid phase. The mushy region is a phase where, in an intimate mixture (grains, dentrites), the two phases can co-exist. Specific microscopic models are used to describe this region in details and this is out of the scope of this presentation. Several authors have studied cicumstances of appearance and disappearance of this mushy region, and after some time if typically disappears.

The geometric interpretation of the Stefan problem arises for the phase transition between liquid ans solid, away from a mushy region. That means at the points of interface $\Gamma(t)$ between the two sets $\Omega_s(t)$ and $\Omega_l(t)$. These are discontinuity points where $w$ jumps form 0 to $\lambda$. Denoting the normal at a point $x$ of the interface $\Gamma(t)$ by $\nu(t,x)$, it moves with a velocity proportional to the jump of normal derivatives according to the law

$$\lambda\, \sigma(t,x) = [[\, d\frac{\partial w}{\partial \nu}\, ]] := d_1 \frac{\partial w}{\partial \nu}|_{x\in\Omega_l} - d_2 \frac{\partial w}{\partial \nu}|_{x\in\Omega_s}. \tag{11.17}$$

## 11.5 Fisher/KPP system with strong competition

$$\begin{cases} \frac{\partial}{\partial t}u(t,x) - d_1\Delta u(t,x) = au(1-u) - kuv, \quad t\geq 0,\ x\in\Omega\subset\mathbb{R}^d, \\ \frac{\partial}{\partial t}v(t,x) - d_2\Delta v(t,x) = bv(1-v) - \alpha kuv, \end{cases} \tag{11.18}$$

The first interesting question is $k \to \infty$ and certainly the second is $d_1 = d_2 = \varepsilon$ and $a = b = 1/\varepsilon$, $k = 1/\varepsilon^2$.

As $k\to\infty$ we obtain the Stefan problem with zero latent heat, with $w = \alpha u - v$

$$\begin{cases} uv = 0, \\ \frac{\partial}{\partial t}u(t,x) - d_1\Delta u(t,x) \leq au(1-u), \\ \frac{\partial}{\partial t}v(t,x) - d_2\Delta v(t,x) \leq bv(1-v), \\ \frac{\partial}{\partial t}w(t,x) - \Delta[d_1 w_+ + d_2 w_-] = G(w), \end{cases} \tag{11.19}$$

with $G(w) = a\frac{w_+}{\alpha}(1-\frac{w_+}{\alpha}) + bw_-(1-w_-)$.

# Chapter 12

# Vanishing diffusion and the Hamilton-Jacobi equation

## 12.1 A linear example; the Hopf-Cole transform

The simplest example of small diffusion limit is when $\varepsilon$ vanishes in the parabolic Lotka-Volterra equation

$$\begin{cases} \frac{\partial}{\partial t}u - \varepsilon^2 \Delta u = uR(x), \qquad t \geq 0, \ x \in \mathbb{R}, \\ u(t=0,x) = u^0(x) > 0, \end{cases}$$

where the growth rate $R(x)$ accounts for birth and death and has apriori no definite sign.

The limit $\varepsilon \to 0$ is borrying because we can expect that the solution converges to that of the ordinary differential system obtained with $\varepsilon = 0$. Therefore, one also re-scale time according to the *diffusion scale* ($X = \sqrt{T}$) to obtain

$$\begin{cases} \varepsilon \frac{\partial}{\partial t}u_\varepsilon - \varepsilon^2 \Delta u_\varepsilon = u_\varepsilon R(x), \qquad t \geq 0, \ x \in \mathbb{R}, \\ u_\varepsilon(t=0,x) = u_\varepsilon^0(x) > 0, \end{cases} \tag{12.1}$$

In the zones where $R$ is positive we expect exponential growth, in the zones where $R$ is negative we expect exponential decay. Therefore the limit $u_\varepsilon$ is not well defined. But the formal expansion $u_\varepsilon(t,x) \approx u_\varepsilon^0 e^{R(x)/\varepsilon}$ suggests to change variable and set

$$u_\varepsilon(t,x) = e^{\varphi_\varepsilon(t,x)/\varepsilon}, \qquad \varphi_\varepsilon(t,x) = \varepsilon \ln\big(u_\varepsilon(t,x)\big). \tag{12.2}$$

The chain rule gives

$$\frac{\partial}{\partial t}u_\varepsilon = \frac{1}{\varepsilon} e^{\varphi_\varepsilon(t,x)/\varepsilon} \frac{\partial}{\partial t}\varphi_\varepsilon(t,x),$$

$$\Delta u_\varepsilon = \frac{1}{\varepsilon} e^{\varphi_\varepsilon(t,x)/\varepsilon} \Delta\varphi_\varepsilon(t,x) + \frac{1}{\varepsilon^2} e^{\varphi_\varepsilon(t,x)/\varepsilon} |\nabla\varphi_\varepsilon(t,x)|^2.$$

Inserting these in the parabolic equation (12.1) gives

$$\begin{cases} \frac{\partial}{\partial t}\varphi_\varepsilon(t,x) - \varepsilon\Delta\varphi_\varepsilon(t,x) - |\nabla\varphi_\varepsilon(t,x)|^2 = R(x), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \varphi_\varepsilon(t=0,x) = \varphi_\varepsilon^0(x). \end{cases} \tag{12.3}$$

The theory of *viscosity solutions* has been developed to handle this limit. We can pass to the limit as a regular perturbation and under suitable assumptions, it can be proved that $\varphi_\varepsilon \underset{\varepsilon\to 0}{\longrightarrow} \varphi$ locally uniformly and this limit satisfies the Hamilton-Jacobi equation

$$\begin{cases} \frac{\partial}{\partial t}\varphi(t,x) = |\nabla\varphi(t,x)|^2 + R(x), \qquad t \geq 0,\ x \in \mathbb{R}, \\ \varphi(t=0,x) = \varphi^0(x). \end{cases} \tag{12.4}$$

This dynamics defines the function $\varphi(t,x)$ which tells us the important, but rough, information on the behavior of $u_\varepsilon(t,x)$. When $\varphi(t,x) > 0$ then $u_\varepsilon(t,x)$ grows exponentially, when $\varphi(t,x) < 0$ then $u_\varepsilon(t,x)$ decays exponentially.

The weakness of this approach is that when $\varphi(t,x) = 0$, we have no information on $u_\varepsilon(t,x)$. More generally when $u_\varepsilon(t,x) = O(1)$ then $\varphi_\varepsilon(t,x) = O(\varepsilon)$ and we do not obtain any relevant information.

## 12.2 A priori Lipschitz bounds

## 12.3 Dirac concentrations

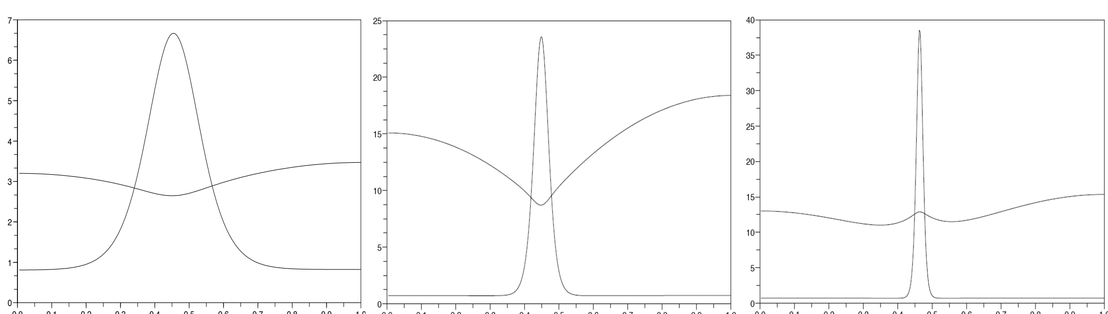

Figure 12.1: Numerical steady state solution of the Brusselator system (7.21) with $A = B = 2$, $d_v = 1.$ and, from left to right $d_u = 0.005$, $d_u = 0.0005$ and $d_u = 0.0001$. The first component $u(x)$ concentrates more and more while $v$ (magnified for plotting) remains flat.

# Chapter 13

# Mathematical tools

## 13.1 Lions-Aubin lemma for time compactness

## 13.2 Michel Pierre's duality estimate

Consider the problem

$$\begin{cases} \frac{\partial}{\partial t} u - \Delta[a(t,x)u] = 0, & x \in \Omega,\ t \geq 0, \\ u(t=0) = u^0, \end{cases}$$

together with Neumann boundary condition in a bounded domain $\Omega$. We denote $Q_T = (0,T) \times \Omega)$. We assume that $a(t,x) > 0$ is smooth and $u$ is a weak solution. We can also assume without lack of generality that $\langle u^0 \rangle \geq 0$. Then we have the a priori estimate

**Lemma 13.1** *For any $T > 0$, we have*

$$\|\sqrt{a}\, u\|_{L^2(Q_T)} \leq C(\Omega)\|u^0\|_{L^2(\Omega)} + 2\langle u^0 \rangle \|\sqrt{a}\|_{L^2(Q_T)}, \tag{13.1}$$

*where $C(\Omega)$ is the constant of Poincaré Wirtinger's inequality.*

**Proof**. Consider smooth functions $F(t,x)$ and the solutions to the adjoint problem

$$\begin{cases} \partial_t v + a(t,x)\Delta v = F(t,x), & x \in \Omega,\ t \leq T, \\ v(t=T) = 0, \end{cases} \tag{13.2}$$

still with Neumann conditions. We have

$$\frac{d}{dt}\int_\Omega uv = \int_\Omega Fu,$$

and thanks to the final condition for the adjoint problem,

$$-\int_\Omega u^0 v^0 = \int_0^T \int_\Omega F u. \tag{13.3}$$

Multiplying (13.2) by $\Delta v$, we get

$$\int_\Omega \partial_t v \Delta v + \int_\Omega a|\Delta v|^2 = \int_\Omega F\Delta v.$$

Integrating by parts on $\Omega$, we obtain,

$$-\frac{d}{dt}\int_\Omega \frac{|\nabla v|^2}{2} + \int_\Omega a|\Delta v|^2 \leq \int_\Omega \left(\frac{F^2}{2a} + \frac{a}{2}|\Delta v|^2\right),$$

which gives after integration in time, using again $v(T) = 0$,

$$\int_\Omega |\nabla v^0|^2 + \int_0^T \int_\Omega a|\Delta v|^2 \leq \int_0^T \int_\Omega \frac{F^2}{a},$$

and by consequence,

$$\|\nabla v^0\|_{L^2(\Omega)} \leq \|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)}, \tag{13.4}$$

$$\|\sqrt{a}\Delta v\|_{L^2(Q_T)} \leq \|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)}. \tag{13.5}$$

We need additionally a bound on $\int v^0$ that we derive as follows. We use again (13.2) to find

$$|\int_\Omega v^0| = |\int_0^T \int_\Omega a\Delta v - F| \leq \int_0^T \int_\Omega \sqrt{a}\Big(\sqrt{a}|\Delta v| + \frac{F}{\sqrt{a}}\Big),$$

which gives, thanks to the Cauchy-Schwarz inequality and (13.5),

$$\left|\int_\Omega v^0\right| \leq 2\|\sqrt{a}\|_{L^2(Q_T)}\|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)}. \tag{13.6}$$

Finally, we get using Poincaré-Wirtinger inequality, (13.6) and then (13.4),

$$\begin{aligned}
\left|\int_\Omega u^0 v^0\right| &\leq \left|\int_\Omega u^0(v^0 - \langle v^0\rangle)\right| + |\int_\Omega \langle u^0\rangle v^0| \\
&\leq C(\Omega)\|u^0\|_{L^2(\Omega)}\|\nabla v^0\|_{L^2(\Omega)} + 2\langle u^0\rangle\|\sqrt{a}\|_{L^2(Q_T)}\|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)} \\
&\leq C(\Omega)\|u^0\|_{L^2(\Omega)}\|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)} + 2\langle u^0\rangle\|\sqrt{a}\|_{L^2(Q_T)}\|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)}.
\end{aligned}$$

Back to (13.3), we conclude that

$$\left|\int_0^T \int_\Omega Fu\right| = \left|\int_0^T \int_\Omega \frac{F}{\sqrt{a}}\sqrt{a}u\right| \leq \Big(C(\Omega)\|u^0\|_{L^2(\Omega)} + 2\langle u^0\rangle\|\sqrt{a}\|_{L^2(Q_T)}\Big)\|\frac{F}{\sqrt{a}}\|_{L^2(Q_T)},$$

which is equivalent to (13.1). $\square$

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