Asymptotic PDE Models for Chemical Reactions and Diffusions

by

Peyam Ryan Tabrizian

A dissertation submitted in partial satisfaction of the

requirements for the degree of

Doctor of Philosophy

in

Mathematics

in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Lawrence C. Evans, Chair Professor Andrew Packard Professor Per-Olof Persson Professor Fraydoun Rezakhanlou

Spring 2016

Asymptotic PDE Models for Chemical Reactions and Diffusions

Copyright 2016 by Peyam Ryan Tabrizian

Abstract

Asymptotic PDE Models for Chemical Reactions and Diffusions

by

Peyam Ryan Tabrizian Doctor of Philosophy in Mathematics University of California, Berkeley Professor Lawrence C. Evans, Chair

In this dissertation, I provide a fairly simple and direct proof of the asymptotics of the scaled Kramers-Smoluchowski equation in one dimension. I further generalize this result to the cases where the potential function H(1) has three or more wells, (2) is periodic, and (3) has infinitely many wells.

I dedicate this thesis to my parents Ali and Feri, to my sister Parissa, to my grandmother Anna, to my aunt Firuse, and to my advisor Professor Lawrence C. Evans, without whom none of this would have been possible. Thank you for your continued support.

Contents

Contents			ii	
List of Figures				
1	The	basic two-well model	1	
	1.1	A model for a simple chemical reaction	1	
	1.2	The Kramers-Smoluchowski equation	3	
	1.3	Goal of this dissertation	4	
	1.4	More detailed discussion of the chemical model	5	
	1.5	Basic estimates	12	
	1.6	Study of the density σ^ϵ	13	
	1.7	A compactness lemma	17	
	1.8	Main theorem	20	
	1.9	Proof of the main theorem	21	
	1.10	Comparison with other methods of proof $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	31	
2	АТ	riple Well–Model	37	
	2.1	Introduction	37	
	2.2	Estimates	38	
	2.3	Main theorem	39	
	2.4	Generalization	44	
3	Peri	odic Wells	48	
-	3.1	Introduction	48	
	3.2	Estimates	48	
	3.3	Main theorem	51	
4	Infinitely-many wells 58			
	4.1	Introduction	58	
	4.2	Estimates	59	
	4.3	Main theorem	60	
Bil	Bibliography			

Bibliography

List of Figures

A double-well potential H	2
Cis-Trans conversion of 2-butene (taken from Moore-Davies-Collins [44])	6
A one-dimensional reduction of the potential surface (taken from Wikipedia [62])	7
Transition state (taken from Wikipedia [61])	8
The cutoff function ψ	22
The functions b^1 and b^2	23
u^{ϵ} exhibiting a boundary layer at 0 $\ldots \ldots \ldots$	34
The smoothing effect of the change of variable $\xi \mapsto s$ (adapted from Arnrich [3])	36
A triple-well potential function H $\dots \dots $	37 40 41 45
A potential H with periodic wells \ldots	49 52
An infinite-well potential H \ldots	58 61
	A double-well potential H

Acknowledgments

I adapted section 1.1 of Chapter 1 from the works of Peletier, Savaré, and Veneroni [48], and sections 1.5 - 1.8 from the paper by Herrmann and Niethammer [29]. Section 1.4 is adapted from the book by McNaught and Wilkinson [40] for the chemical terminology and from the book by Risken [52] for the derivation of the Kramers-Smoluchowski equation (1.3).

Chapter 1

The basic two–well model

1.1 A model for a simple chemical reaction

Consider a simple chemical reaction $A \rightleftharpoons B$, where a molecule A transforms into B and vice-versa. For example, think of A and B as two forms of the same molecule with spatial asymetry and which therefore exists in two distinct mirror-like spatial configurations.

On the one hand, denoting by $\alpha = \alpha(x, t)$ the volume fraction of A and by $\beta = \beta(x, t)$ the volume fraction of B (so that $\alpha + \beta = 1$), using a chemical modeling argument (cf. section 1.4), one obtains that α and β solve the reaction-diffusion system

$$\begin{cases} \alpha_t - a_{-1}\Delta\alpha = \kappa \left(\beta - \alpha\right) \\ \beta_t - a_1\Delta\beta = \kappa \left(\alpha - \beta\right), \end{cases}$$
(1.1)

where $a_{\pm 1}$ are diffusion constants and κ is the rate constant of the reaction, assumed to be the same for both reactions $A \to B$ and $B \to A$. Here, and throughout the rest of the dissertation, $\Delta = \Delta_x$ denotes the Laplacian in the *x*-variable and $\nabla = \nabla_x$ the gradient in the *x*-variable.

On the other hand, one can augment (1.1) by adding a one-dimensional chemical variable ξ that represents the different arrangements of the atoms inside the molecule (while, in contrast, x represents the spatial degrees of freedom of the molecule). We assume that the energy of a state (x, ξ) is given by a potential function $H = H(\xi)$ that is independent of x and that has a double-well structure, as in Figure 1.1 on the next page. Here, $\xi = -1$ corresponds to the stable state A and $\xi = 1$ to the stable state B, with infinitely many (unstable) states in between. In that case, the molecule undergoes an SDE driven by H and Gaussian noise, and its probability distribution $\rho^{\epsilon} = \rho^{\epsilon}(x, \xi, t)$ satisfies the Kramers-Smoluchowski equation



Figure 1.1: A double-well potential H

$$\tau_{\epsilon} \left(\rho_{t}^{\epsilon} - a^{\epsilon} \Delta \rho^{\epsilon} \right) = \left(\rho_{\xi}^{\epsilon} + \epsilon^{-2} \rho^{\epsilon} H' \right)_{\xi}.$$

$$(1.2)$$

Here τ_{ϵ} is an appropriate scaling factor in time that provides a nontrivial asymptotic limit of the system, and a^{ϵ} is the diffusion-coefficient. The quantity $\frac{1}{\epsilon}$ is interpreted as an activation energy; so the limit as $\epsilon \to 0$ corresponds to a limit of large activation energy, where the energy barrier separating the two wells of H is large compared to the noise.

The following question then arises: How are (1.1) and (1.2) related? Are they two sides of the same coin? Is it possible to take a limit of large activation energy such that the solutions of (1.2) converge to (1.1)?

The Kramers-Smoluchowski equation (1.2) has been studied since the 1930s in the context of chemical reaction rates. In that context, a molecule can be thought of as a particle moving in a high-dimensional potential landscape H, driven by fluctuations and Gaussian noise; a chemical reaction then corresponds to the movement of that particle from one minimum of the potential to the other. The potential H is the solution of a Schrödinger equation, which is in practice impossible to solve explicitly, except in the case of the hydrogen atom. That said, the Born-Oppenheimer approximation [13] in quantum mechanics, which is a kind of a separation of variables, provides us with an 'approximate' potential H by treating the nucleus of the particle as fixed, and solving the Schrödinger equation for the electrons only. Using this approximate potential, the chemical reaction rate then follows from a SDE, from which Kramers [34] derived its Fokker-Planck equation and studied its large friction-limit, whose corresponding equation is

$$\rho_t - \Delta \rho - (\rho_{\xi} + \rho H')_{\xi} = 0.$$

However, even in this situation, the reaction rate is impossible to calculate explicitly, and instead effort has been directed in determining the reaction rates in a special case, where the energy barrier separating the two wells is very large. This is called the limit of large activation energy and leads to (1.2). There are many successful results in this direction; see the paper by Hänggi [27] and the paper by Berglund [11] for an overview, and consult the book by Hehre [28] for a general survey of quantum chemical models. In section 1.4, we will elaborate the chemical background even further and in particular explain how Kramers derived (1.3) from an SDE.

1.2 The Kramers-Smoluchowski equation

In this dissertation, we investigate the behavior as $\epsilon \to 0$ of solutions ρ^{ϵ} of the **Kramers-Smoluchowski** equation

$$\begin{cases} \tau_{\epsilon} \left(\rho_{t}^{\epsilon} - a^{\epsilon} \Delta \rho^{\epsilon}\right) = \left(\rho_{\xi}^{\epsilon} + \epsilon^{-2} \rho^{\epsilon} H'\right)_{\xi} & \text{in } U \times \mathbb{R} \times [0, T] \\ \frac{\partial \rho^{\epsilon}}{\partial \nu} = 0 & \text{on } \partial U \times \mathbb{R} \times [0, T] \\ \rho^{\epsilon} = \rho_{0}^{\epsilon} & \text{on } U \times \mathbb{R} \times \{t = 0\} \,. \end{cases}$$
(1.3)

Here U is an open and bounded domain in \mathbb{R}^n , with smooth boundary ∂U , $D := U \times \mathbb{R}$,

 $\rho^\epsilon=\rho^\epsilon(x,\xi,t)$ is the density of a probability measure, with given initial condition $\rho^\epsilon_0=\rho^\epsilon(x,\xi,0)\geq 0,$

 $\tau_{\epsilon} := \frac{1}{\epsilon^2} e^{-\frac{1}{\epsilon^2}}$ is a scaling in time that will give a nontrivial asymptotic limit,

 $a^{\epsilon} = a^{\epsilon}(\xi) \in C(\mathbb{R})$ is a diffusion-coefficient, with $a^{\epsilon} \ge \theta > 0$, for some constant θ independent of ϵ , and

 $H = H(\xi)$ is a smooth, nonnegative, and even double-well potential function with H(0) = H(2) = 1, H(1) = 0, a local maximum at 0 and a local minimum at 1, and H is de-

creasing on (0,1) and increasing on $(1,\infty)$. Thus H has the W-shape as drawn in Figure 1.1.

We will often switch between the measure-theoretic formulation of (1.3) and the functional formulation (1.4) below. More precisely, define

$$\sigma^{\epsilon} := e^{\frac{\bar{H}_{\epsilon} - H}{\epsilon^2}}$$
, where \bar{H}_{ϵ} is chosen so that $\int_{\mathbb{R}} \sigma^{\epsilon} d\xi = 1$,

and let

$$u^{\epsilon}(x,\xi,t) := \frac{\rho^{\epsilon}(x,\xi,t)}{\sigma^{\epsilon}(\xi)}.$$

Then (1.3) becomes

$$\begin{cases} \sigma^{\epsilon} \left(u_{t}^{\epsilon} - a^{\epsilon} \Delta u^{\epsilon} \right) = \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} & \text{in } U \times \mathbb{R} \times [0, T] \\ \frac{\partial u^{\epsilon}}{\partial \nu} = 0 & \text{on } \partial U \times \mathbb{R} \times [0, T] \\ u^{\epsilon} = u_{0}^{\epsilon} := \frac{\rho_{0}^{\epsilon}}{\sigma^{\epsilon}} & \text{on } U \times \mathbb{R} \times \{t = 0\} \,. \end{cases}$$

$$(1.4)$$

1.3 Goal of this dissertation

Our goal is to study the limits as $\epsilon \to 0$ of ρ^{ϵ} and u^{ϵ} in (1.3) and (1.4). Here and throughout this dissertation, we will denote $\delta_i := \delta_{\{\xi=i\}}$ and $a_i := a(i)$ (where $i \in \mathbb{R}$). We will show that, under certain assumptions on the initial condition u_0^{ϵ} and diffusion coefficient a^{ϵ} , and, in a precise sense given later,

$$\rho^{\epsilon} \stackrel{\star}{\rightharpoonup} \alpha \, \delta_{-1} + \beta \, \delta_1$$

for some functions $\alpha = \alpha(x,t)$ and $\beta = \beta(x,t)$ which satisfy the system of reactiondiffusion equations in $U \times [0,T]$

$$\begin{cases} \alpha_t - a_{-1}\Delta\alpha &= \kappa \left(\beta - \alpha\right) \\ \beta_t - a_1\Delta\beta &= \kappa \left(\alpha - \beta\right), \end{cases}$$
(1.5)

where

$$\kappa := \frac{\sqrt{|H''(0)| H''(1)}}{2\pi}$$

is the corresponding rate constant of the chemical reaction $A \rightleftharpoons B$.

Previous work and outline

The relationship between (1.3) and (1.5) has already been studied in previous papers. In [48], Peletier et al. rewrite both (1.3) and (1.5) in terms of variational evolution equations, and prove that the quadratic form associated to (1.3) Γ -converges to the one associated to (1.5). In a later paper [29], Herrmann and Niethammer provide a novel proof of the same problem, rewriting (1.3) as a gradient flow on the Wasserstein space of probability measures and using an integrated Raleigh-principle. Finally, Arnrich et. al. [3] give a proof of the same result, but this time using the Wasserstein structure of the two equations only. The proofs given in those three papers will be outlined later, in section 1.10.

While both approaches give new and interesting insights into the problem, this dissertation provides a more direct proof of the same result. It is based on multiplying (1.4) by clever test functions $\phi^{1,\epsilon}$ and $\phi^{2,\epsilon}$ which effectively cancel out the singular term $\sigma^{\epsilon}/\tau_{\epsilon}$. Our approach allows one to adapt the same proof to more complicated models, some of which are studied in the latter portion of this dissertation. We will examine the cases where (1) H has 3 wells, (2) H is periodic, and (3) H has infinitely many wells. Moreover, in a forthcoming paper with Lawrence C. Evans [21], we even provide a generalization to the case where ξ is more than one-dimensional.

1.4 More detailed discussion of the chemical model

This section discusses some of the chemical quantities in play in more detail, and provides a derivation of (1.3) from a general Fokker-Planck equation, and a derivation of (1.5) from a more elementary reaction rate equation. For more information on the chemical background, consult the book by McNaught and Wilkinson [40] (sometimes called the 'Gold Book').

The chemical variable ξ

The variable ξ is called a reaction-coordinate and represents progress of the chemical reaction $A \rightleftharpoons B$ along the reaction-pathway from A to B. It usually, but not always, represents an actual physical quantity such as the length of a bond or angle of a bond. For example, in the reaction diagram (Figure 1.2) on the next page, which models the conversion from Cis-2-butene to Trans-2-butene, ξ represents the angle of twist of the 2-butene molecule, ranging from -30° to 210° .



Figure 1.2: Cis-Trans conversion of 2-butene (taken from Moore-Davies-Collins [44])

The potential function H

In our context, the potential H represents the Gibbs free energy of a molecule (usually denoted by G in the chemical literature) as a function of its chemical variable ξ . In theory, the variable ξ in H could be multi-dimensional, as in the case of a molecule that can twist in many different directions, or in the case of the water-molecule, where $\xi = (\xi_1, \xi_2)$, with ξ_1 being the length of the bond O - H, and ξ_2 being the bond angle H - O - H. For practical purposes, however, one may reduce ξ to a single variable, by imagining a curve that connects two energy minima in the direction that traverses the minimum energy barrier (cf. the book by Lewars [36]), as depicted in the Figure 1.3 on the next page. Note that the minimum transition cost K^{ϵ} in Peletier et. al. [48] is a rigorous mathematical formulation of this idea (see section 1.10 below).

The Gibbs free energy H is defined as



Figure 1.3: A one-dimensional reduction of the potential surface (taken from Wikipedia [62])

$$H = U + pV - TS.$$

where U is the internal energy of the system, p the pressure (assumed to be constant), V the volume, T the temperature and S the entropy (a measure of the complexity of a system). The term U + pV is sometimes called the enthalpy of the system, so one can think of H as being the difference between the enthalpy and the (scaled) entropy of the system. The significance of H lies within the fact that a chemical reaction occurs if and only if the change ΔH in the Gibbs energy is less than the change $\Delta W := p\Delta V$ of non-Pressure-Volume work (which is usually 0). Therefore, one way to induce a chemical reaction then is to either break the bonds of a molecule (which decreases U), or to increase the temperature T. A system with $\Delta H = 0$, such as the one that we are considering, is in an equilibrium state.

Transition-state theory

The maximum of H is called a transition state. Transition-state theory was pioneered by Eyring, and Evans-Polanyi (see the paper by Laidler and King [35] for an overview) and can be used to calculate the rate constant κ via the differential equation



Reaction Coordinate

Reaction: $HO^- + CH_3Br \rightarrow [HO---CH_3---Br]^+ \rightarrow CH_3OH + Br^-$

Figure 1.4: Transition state (taken from Wikipedia [61])

$$\frac{d\ln(\kappa)}{dT} = \frac{\Delta G^{\ddagger}}{RT^2},\tag{1.6}$$

where T is the thermodynamic temperature and R is the universal gas constant. The quantity ΔG^{\ddagger} is the change of Gibbs energy between the initial state and the the transition state. It is called the activation energy and it is the minimum energy which must be available to a chemical system to result in a reaction. Figure 1.4 on the next page gives a pictorial representation of the activation energy.

The equation (1.6) has the following solution, called the Arrhenius equation (pioneered by Arrhenius in [4] and adapted here to modern terminology):

$$\kappa = A e^{-\frac{\Delta G^{\ddagger}}{RT}}.$$
(1.7)

In this dissertation, we consider the limit of large activation energy, that is when $\Delta G^{\ddagger} \rightarrow \infty$; This is explains why we rescale the height of H to H/ϵ^2 in (1.3). In theory, this would imply that $\kappa = 0$ in (1.7), but it is precisely the choice of $\tau_{\epsilon} = \frac{1}{\epsilon^2} e^{-\frac{1}{\epsilon^2}}$ that will avoid such a degeneracy and give us a nontrivial limit of κ .

Derivation of the Kramers-Smoluchowski equation (1.3)

As explained in the book by Risken [52], the equation (1.3) is part of a more general class of Fokker-Planck equations, which are equations of the form

$$\rho_t = -\sum_{i=1}^n \left(b^i(\mathbf{x}) \rho \right)_{x_i} + \sum_{i,j=1}^n \left(a^{ij}(\mathbf{x}) \rho \right)_{x_i x_j}, \qquad (1.8)$$

where $\mathbf{x} \in \mathbb{R}^n$ and $A = [a^{ij}]$ is an $n \times n$ matrix satisfying the ellipticity condition

$$\sum_{i,j=1}^{n} a^{ij}(\mathbf{x})\xi_i\xi_j \ge 0$$

for all $\mathbf{x} \in \mathbb{R}^n$ and all $\boldsymbol{\xi} = (\xi_1, \cdots, \xi_n) \in \mathbb{R}^n$.

There is a close link between Fokker-Planck equations (1.8) and SDE. Namely, if $\mathbf{X}_t \in \mathbb{R}^n$ is a stochastic process satisfying the SDE

$$d\mathbf{X}_t = \boldsymbol{\mu}(\mathbf{X}_t, t)dt + \boldsymbol{\sigma}(\mathbf{X}_t, t)d\mathbf{B}_t, \qquad (1.9)$$

where $\boldsymbol{\mu} = (\mu^1, \dots, \mu^n)$ is a *n*-dimensional random vector, $\boldsymbol{\sigma} = [\sigma^{ij}]$ is a $n \times m$ random matrix, and \mathbf{B}_t denotes *m*-dimensional Brownian motion, then the probability density $\rho(\mathbf{x}, t)$ for \mathbf{X}_t satisfies the Fokker-Planck equation

$$\rho_t = -\sum_{i=1}^n \left(\mu^i \rho\right)_{x_i} + \frac{1}{2} \sum_{i,j=1}^n \left(D^{ij} \rho\right)_{x_i x_j},\tag{1.10}$$

where

$$D^{ij} := \sum_{k=1}^m \sigma^{ik} \sigma^{jk}$$

Note that in the simple one-dimensional (n = 1) Brownian motion-case

$$dX_t = dB_t,$$

which corresponds to $\mu = 0$ and $\sigma = 1$, we recover the usual (scaled) heat-equation

$$\rho_t = \frac{1}{2}\Delta\rho.$$

In order to derive (1.3), Kramers, in his original paper [34], studied the following scenario: Consider a set of particles subject to Brownian motion with their distribution function $\rho = \rho(x, v, t)$ at position x, velocity v, and time t, satisfying the Kramers equation

CHAPTER 1. THE BASIC TWO-WELL MODEL

$$\rho_t = -\rho_x + \left[\left(\gamma v - \frac{F(x)}{m} \right) \rho \right]_v + \frac{\gamma kT}{m} \rho_{vv}, \qquad (1.11)$$

where γ is the friction constant, m the mass of the particle, T the temperature of the fluid, k the Boltzmann constant, mf(x) the potential with F(x) = -mf'(x) the external force. This is indeed of the form (1.8) with n = 2, $\mathbf{x} = (x, v) \in \mathbb{R}^2$, $\mathbf{b} = (1, \frac{F}{m} - \gamma v) a^{11} = a^{12} = a^{21} = 0$, $a^{22} = \frac{\gamma kT}{m}$. Moreover, it can be written in the form (1.10), with m = n = 2, $\boldsymbol{\mu} = (1, \frac{F}{m} - \gamma v)$ and $\sigma^{11} = \sigma^{12} = \sigma^{21} = 0$, $\sigma^{22} = \sqrt{\frac{2\gamma kT}{m}}$. The SDE (1.9) corresponding to (1.11) is then

$$\begin{cases} dx = v \, dt \\ dv = \left(\frac{F(x)}{m} - \gamma v\right) \, dt + \sqrt{\frac{2\gamma kT}{m}} dB_t, \end{cases}$$
(1.12)

which can be written more compactly as

$$m\ddot{x} + m\gamma\dot{x} = F(x) + \sqrt{2\gamma kTm}B_t, \qquad (1.13)$$

where \dot{x} denotes the time-derivative of x. Now in the so-called large friction-limit, when γ is large, we can ignore \ddot{x} in (1.13), thereby obtaining the SDE

$$dx = \frac{F(x)}{m\gamma}dt + \sqrt{\frac{2kT}{m\gamma}}dB_t,$$
(1.14)

which corresponds to m = n = 1, $\mu = \frac{F(x)}{m\gamma}$ and $\sigma = \sqrt{\frac{2kT}{m\mu}}$ in (1.9). The corresponding Fokker-Planck equation (1.10) for the distribution function $\rho = \rho(x, t)$ in the (x, t)-variables only is then

$$\rho_t = -\left(\frac{F(x)}{m\gamma}\rho\right)_x + \frac{kT}{m\gamma}\rho_{xx}$$

In our problem, setting $m = 1, k = 1, T = 1, \gamma = \tau_{\epsilon}$, and $f(x) = H/\epsilon^2$, so $F(x) = -H'/\epsilon^2$, and writing ξ instead of x, we indeed obtain (1.3) (without the spatial diffusion term).

Derivation of the reaction-diffusion system (1.5)

The system (1.5) is derived from the rate equation for chemical reactions. For sake of simplicity, we will suppress the x-dependency of the quantities in question. For the general reaction $aA + cC \rightleftharpoons bB + dD$, the reaction rate r is defined as

$$r = \kappa_1 [A]^a [C]^c - \kappa_2 [B]^b [D]^d, \qquad (1.15)$$

where κ_1 and κ_2 are the rate constants for the forward and backward reactions, that is, all the parameters other than concentration (such as temperature) that affect r. The usefulness of the reaction rate r lies in the rate equation, which states that

$$r = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{c}\frac{d[C]}{dt} = \frac{1}{b}\frac{d[B]}{dt} = \frac{1}{d}\frac{d[D]}{dt}.$$

This intuitively tells use that r measures how fast the concentrations of the reactants A and C and products C and D change during the reaction.

The unimolecular case $A \rightleftharpoons B$ corresponds to the case a = b = 1 and c = d = 0; moreover, in this dissertation, we assume that $\kappa_1 = \kappa_2 := \kappa$. Therefore, denoting [A] and [B] as α and β , the above expression (1.15) for r simplifies to

$$r = \kappa \alpha - \kappa \beta = \kappa (\alpha - \beta),$$

and $-\frac{d[A]}{dt} = r$ is equivalent to

$$\alpha_t = -r = \kappa(\beta - \alpha), \tag{1.16}$$

and $\frac{d[B]}{dt} = r$ reduces to

$$\beta_t = r = \kappa(\alpha - \beta). \tag{1.17}$$

The equations (1.16) and (1.17) then give us the desired reaction-diffusion system (1.5).

More general reaction-diffusion systems

Reaction-diffusion systems like (1.5) arise in a wide array of mathematical models, such as the spread of biological populations (see the original paper by Fisher [23], and also the works of Berestycki et. al. [10] and [9]), the propagation of flames in combustion theory (Zeldovich et. al. [63]), the blocking of neural networks (see again the works of Berestycki et. al. [8]), blood clotting (Lobanova et. al. [38]), and a model for gases (Purwins [50]). They generally exhibit a wide range of behaviors, including the formation of traveling waves, as well as pattern-formation such as stripes or hexagons, or more intricated structures like dissipative solutions. An overview of the range of possible phenomena is given in the book by Liehr [37]. They are also of interest mathematically because, although they are generally nonlinear, they are usually well-posed. Consult the books by Fife [22], Grindrod [26], Kerner et. al. [33], Mikhailov [43], and Smoller [56] for an overview of the theory of reaction-diffusion equations.

Basic estimates 1.5

Let us begin by stating and proving two regularization estimates.

Lemma 1. For all $0 \le t \le T$,

$$\int_{D} \frac{\sigma^{\epsilon}}{2} \left| u^{\epsilon}(x,\xi,t) \right|^{2} dx d\xi + \int_{0}^{t} \int_{D} \left(\sigma^{\epsilon} a^{\epsilon} \left| \nabla u^{\epsilon}(x,\xi,s) \right|^{2} + \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u^{\epsilon}_{\xi}(x,\xi,s) \right|^{2} \right) dx d\xi ds = \int_{D} \frac{\sigma^{\epsilon}}{2} \left| u^{\epsilon}(x,\xi,0) \right|^{2} dx d\xi. \quad (1.18)$$

Proof. Multiply (1.4) by u^{ϵ} and integrate over $D \times [0, t]$ to get

$$\int_0^t \int_D \sigma^\epsilon u_t^\epsilon u^\epsilon dx d\xi ds - \int_0^t \int_D \sigma^\epsilon a^\epsilon (\Delta u^\epsilon) u^\epsilon dx d\xi ds = \int_0^t \int_D \left(\frac{\sigma^\epsilon}{\tau_\epsilon} u_\xi^\epsilon\right)_\xi u^\epsilon dx d\xi ds.$$
(1.19)

Because $u_t^{\epsilon} u^{\epsilon} = \frac{1}{2} \partial_t |u^{\epsilon}|^2$, the first term on the left-hand-side of (1.19) becomes

$$\int_0^t \int_D \sigma^\epsilon u_t^\epsilon u^\epsilon dx d\xi dt = \frac{1}{2} \int_D \sigma^\epsilon |u^\epsilon(x,\xi,t)|^2 dx d\xi - \int_D \sigma^\epsilon |u^\epsilon(x,\xi,0)|^2 dx d\xi.$$
(1.20)

Now after integrating by parts with respect to x and using $\frac{\partial u^{\epsilon}}{\partial \nu} = 0$ on $\partial U \times \mathbb{R} \times [0, t]$, the second term on the left-hand-side of (1.19) equals to

$$-\int_0^t \int_D \sigma^\epsilon a^\epsilon (\Delta u^\epsilon) u^\epsilon dx d\xi ds = \int_0^t \int_D \sigma^\epsilon a^\epsilon |\nabla u^\epsilon(x,\xi,s)|^2 dx d\xi ds.$$
(1.21)

Similarly, integrating by parts with respect to ξ , the term on the right of (1.19) can be written as

$$\int_{0}^{t} \int_{D} \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} u^{\epsilon} dx d\xi ds = \int_{0}^{t} \int_{D} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u_{\xi}^{\epsilon}(x,\xi,s) \right|^{2} dx d\xi ds.$$
(1.22)
vs from (1.20) - (1.22) applied to (1.19).

The result follows from (1.20) - (1.22) applied to (1.19).

Lemma 2. For all $0 \le t \le T$,

$$\frac{1}{2} \int_{D} \left(\sigma^{\epsilon} a^{\epsilon} \left| \nabla u^{\epsilon}(x,\xi,t) \right|^{2} + \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u^{\epsilon}_{\xi}(x,\xi,t) \right|^{2} \right) dx d\xi + \int_{0}^{t} \int_{D} \sigma^{\epsilon} \left| u^{\epsilon}_{t}(x,\xi,s) \right|^{2} dx d\xi ds$$

$$= \frac{1}{2} \int_{D} \left(\sigma^{\epsilon} a^{\epsilon} \left| \nabla u^{\epsilon}(x,\xi,0) \right|^{2} + \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u^{\epsilon}_{\xi}(x,\xi,0) \right|^{2} \right) dx d\xi. \quad (1.23)$$

Proof. This time multiply (1.4) by u_t^{ϵ} and integrate over $D \times [0, t]$ to get

$$\int_{0}^{t} \int_{D} \sigma^{\epsilon} |u_{t}^{\epsilon}|^{2} dx d\xi ds - \int_{0}^{t} \int_{D} \sigma^{\epsilon} a^{\epsilon} (\Delta u^{\epsilon}) u_{t}^{\epsilon} dx d\xi ds = \int_{0}^{t} \int_{D} \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} u_{t}^{\epsilon} dx d\xi ds.$$
(1.24)

Integrating by parts with respect to x, using $\frac{\partial u^{\epsilon}}{\partial \nu} = 0$ on $\partial U \times \mathbb{R} \times [0, t]$ and $\nabla u^{\epsilon} \cdot (\nabla u^{\epsilon})_t = \frac{1}{2} \partial_t |\nabla u^{\epsilon}|^2$, the second term on the left of (1.24) becomes

$$\int_{0}^{t} \int_{D} \sigma^{\epsilon} a^{\epsilon} \left(\Delta u^{\epsilon}\right) u_{t}^{\epsilon} dx d\xi ds = \frac{1}{2} \int_{D} \sigma^{\epsilon} a^{\epsilon} \left|\nabla u^{\epsilon}(x,\xi,t)\right|^{2} dx d\xi - \frac{1}{2} \int_{D} \sigma^{\epsilon} a^{\epsilon} \left|u^{\epsilon}(x,\xi,0)\right|^{2} dx d\xi.$$

$$(1.25)$$

Similarly, integrating by parts with respect to ξ , the term on the right of (1.24) becomes

$$\int_{0}^{t} \int_{D} \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} u_{t}^{\epsilon} dx d\xi ds = \frac{1}{2} \int_{D} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u_{\xi}^{\epsilon}(x,\xi,t) \right|^{2} dx d\xi - \frac{1}{2} \int_{D} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u_{\xi}^{\epsilon}(x,\xi,0) \right|^{2} dx d\xi.$$
(1.26)

The result follows from (1.25) and (1.26) applied to (1.24).

Note: Assumptions (1.37) and (1.38) in the main theorem below in fact assert that the right-hand-sides of (1.18) and (1.23) are bounded from above independently of ϵ .

1.6 Study of the density σ^{ϵ}

In this section, we derive convergence results for σ^{ϵ} and $\frac{\sigma^{\epsilon}}{\tau_{\epsilon}}$, which will allow us later to extract suitable convergent subsequences of ρ^{ϵ} . Before stating those results, let us recall the statement of Laplace's method, a proof of which can be found in Bender-Orszag [7].

Theorem 1 (Laplace's method). If $f = f(\xi)$ is a twice-differentiable function on [a, b] and ξ_0 is the unique minimum point of f with $f''(\xi_0) > 0$, then

$$\int_{a}^{b} e^{\frac{-f(\xi)}{\epsilon^{2}}} d\xi = e^{\frac{-f(\xi_{0})}{\epsilon^{2}}} \left(\frac{2\pi\epsilon^{2}}{f''(\xi_{0})}\right)^{\frac{1}{2}} (1+o(1)) \quad as \ \epsilon \to 0.$$

Note: For an extension to infinite intervals (See again Bender-Orszag [7]), we can take $a = -\infty$ or $b = \infty$ (or both) if we moreover assume that (1) $\int_a^b e^{-f(\xi)} d\xi$ is finite, and (2) $f(\xi_0)$ is a true minimum, i.e. there exist $\delta > 0$ small enough and $\eta > 0$ such that if $|\xi - \xi_0| > \delta$, then $f(\xi) \ge f(\xi_0) + \eta$.

$$\square$$

Using the normalization $\int_{\mathbb{R}} \sigma^{\epsilon} d\xi = 1$, the fact that H is even, and finally Laplace's method applied to $f(\xi) = H(\xi)$ with $a = 0, b = \infty$, and $\xi_0 = 1$, we obtain

$$e^{-\frac{\bar{H}_{\epsilon}}{\epsilon^{2}}} = \int_{\mathbb{R}} e^{-\frac{H(\xi)}{\epsilon^{2}}} d\xi = 2 \int_{0}^{\infty} e^{-\frac{H(\xi)}{\epsilon^{2}}} d\xi = \epsilon \frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} \left(1 + o(1)\right)$$

This gives us the following asymptotic expansion of $e^{\frac{\bar{H}_{\epsilon}}{\epsilon^2}}$:

$$e^{\frac{\bar{H_{\epsilon}}}{\epsilon^2}} = \frac{1}{\epsilon} \frac{\sqrt{H''(1)}}{2\sqrt{2\pi}} (1 + o(1)).$$

To state the compactness estimates, here and in the following, let $\delta = \delta(\epsilon) = \epsilon^{\frac{3}{4}}$. Notice that with this choice of δ , we have that, for all c > 0,

$$\lim_{\epsilon \to 0} \delta = 0, \quad \lim_{\epsilon \to 0} \frac{\delta}{\epsilon} = \infty, \quad \lim_{\epsilon \to 0} \frac{\delta^3}{\epsilon^2} = 0, \quad \lim_{\epsilon \to 0} \epsilon e^{\left(\frac{\delta}{\epsilon}\right)^2} = \infty, \quad \lim_{\epsilon \to 0} \frac{1}{\epsilon} e^{-c\left(\frac{\delta}{\epsilon}\right)^2} = 0.$$
(1.27)

Lemma 3. Define $I_{\delta} := (-1-\delta, -1+\delta) \cup (1-\delta, 1+\delta)$ and $J_{\delta} := (-2-\delta, -2+\delta) \cup (-\delta, \delta) \cup (2-\delta, 2+\delta)$. As $\epsilon \to 0$, we have

$$\sup_{\mathbb{R}\setminus I_{\delta}} \sigma^{\epsilon} \longrightarrow 0, \qquad \int_{\mathbb{R}\setminus I_{\delta}} \sigma^{\epsilon} d\xi \longrightarrow 0, \qquad \int_{\pm 1-\delta}^{\pm 1+\delta} \sigma^{\epsilon} d\xi \longrightarrow \frac{1}{2}, \tag{1.28}$$

$$\inf_{(-2,2)\backslash J_{\delta}} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \longrightarrow \infty, \qquad \int_{2}^{3} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} d\xi \longrightarrow 0, \qquad (1.29)$$

$$\int_{-2,2)\backslash J_{\delta}} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow 0, \qquad \int_{-\delta}^{\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow \frac{2}{\kappa}.$$
(1.30)

Proof. 1. If ϵ and (therefore) δ are small enough, we have, on $\mathbb{R} \setminus I_{\delta}$, that

(

$$H(\xi) \ge \min\left(H(1+\delta), H(1-\delta)\right) \ge \frac{1}{2}H''(1)\delta^2\left(1+o(1)\right)$$
 (by Taylor expansion),

and therefore

$$\begin{aligned} \sigma^{\epsilon} &= e^{\frac{\bar{H}_{\epsilon}-H}{\epsilon^{2}}} \\ &\leq e^{\frac{\bar{H}_{\epsilon}}{\epsilon^{2}}} e^{-\frac{\frac{1}{2}H''(1)\delta^{2}(1+o(1))}{\epsilon^{2}}} \\ &= \frac{1}{\epsilon} \frac{\sqrt{H''(1)}}{2\sqrt{2\pi}} (1+o(1))e^{-\frac{1}{2}H''(1)\left(\frac{\delta}{\epsilon}\right)^{2}(1+o(1))} \\ &= \left(\frac{1}{\epsilon}e^{-\left(\frac{\delta}{\epsilon}\right)^{2}\frac{H''(1)}{2}(1+o(1))}\right)\frac{\sqrt{H''(1)}}{2\sqrt{2\pi}} (1+o(1)) \end{aligned}$$

By (1.27), the term in parentheses goes to 0 as $\epsilon \to 0$, uniformly in ξ . This proves the first part of (1.28).

2. Again by Taylor expansion, if $\xi \in (-\delta, \delta)$, we obtain

$$H(1+\xi) = \frac{1}{2}H''(1)(\xi^2 + O(|\xi|^3)) = \frac{1}{2}H''(1)\xi^2(1+O(|\xi|))$$

Therefore, if δ is small enough,

$$\begin{split} \int_{\pm 1-\delta}^{\pm 1+\delta} \sigma^{\epsilon} d\xi &= e^{\frac{H_{\epsilon}}{\epsilon^{2}}} \int_{-\delta}^{\delta} e^{-\frac{\frac{1}{2}H''(1)\xi^{2}(1+O(|\xi|))}{\epsilon^{2}}} d\xi \\ &= \left(\frac{1}{\epsilon} \frac{\sqrt{H''(1)}}{2\sqrt{2\pi}} (1+o(1))\right) \epsilon \int_{-\frac{\delta}{\epsilon}}^{\frac{\delta}{\epsilon}} e^{-\frac{H''(1)}{2}\xi^{2}(1+O(\epsilon|\xi|))} d\xi \qquad \text{(Change of variables)} \\ &= \frac{1}{2} \sqrt{\frac{H''(1)}{2\pi}} (1+o(1))^{2} \int_{-\frac{\delta}{\epsilon}}^{\frac{\delta}{\epsilon}} e^{-\frac{H''(1)}{2}\xi^{2}} d\xi \\ &\stackrel{\epsilon \to 0}{\longrightarrow} \frac{1}{2} \sqrt{\frac{H''(1)}{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{H''(1)}{2}\xi^{2}} d\xi \\ &= \frac{1}{2} \sqrt{\frac{H''(1)}{2\pi}} \sqrt{\frac{2\pi}{H''(1)}} \qquad \text{(Gaussian integral)} \\ &= \frac{1}{2}. \end{split}$$

The third equality follows because on $(-\delta/\epsilon, \delta/\epsilon)$, $\xi^2 O(\epsilon |\xi|) = O(\delta^3/\epsilon^2) \to 0$ by (1.27), and the fourth one by the Dominated Convergence Theorem and because $\delta/\epsilon \to \infty$, again by (1.27). This proves the third part of (1.28), and the second part follows because $\int_{\mathbb{R}} \sigma^{\epsilon} d\xi = 1$.

3. If $\xi \in (-3,3) \setminus J_{\delta}$, then by Taylor expansion, we get

$$H(\xi) \le \max(H(\delta), H(2-\delta)) \le 1 + o(\delta) - \min\left(\frac{1}{2} |H''(0)| \,\delta^2, H'(2)\delta\right).$$

Therefore

$$\begin{split} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} &= \epsilon^{2} e^{\frac{1}{\epsilon^{2}}} e^{\frac{H_{\epsilon}-H}{\epsilon^{2}}} \\ &\geq \left(\frac{1}{\epsilon} \frac{\sqrt{H''(1)}}{2\sqrt{2\pi}} (1+o(1))\right) \epsilon^{2} e^{\frac{1}{\epsilon^{2}}} e^{\frac{-1+o(\delta)+\min\left(\frac{1}{2}|H''(0)|\delta^{2},H'(2)\delta\right)}{\epsilon^{2}}} \\ &\geq \left(\frac{\sqrt{H''(1)}}{2\sqrt{2\pi}} (1+o(1))\right) \epsilon \min\left(e^{\frac{1}{2}|H''(0)|\left(\frac{\delta}{\epsilon}\right)^{2}}, e^{H'(2)\frac{\delta}{\epsilon^{2}}}\right) e^{\frac{o(\delta)}{\epsilon^{2}}} \\ &\longrightarrow \infty \qquad (by \ (1.27)). \end{split}$$

From this, the first part of (1.29) and the first part of (1.30) follow.

4. Since H is increasing on (2,3), we have $H(\xi) \ge H(2) = 1$ on (2,3), and hence

$$\begin{split} \int_{2}^{3} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} &= \epsilon^{2} e^{\frac{1}{\epsilon^{2}}} e^{\frac{\bar{H}_{\epsilon}}{\epsilon^{2}}} \int_{2}^{3} e^{-\frac{H}{\epsilon^{2}}} d\xi \\ &\leq \epsilon^{2} e^{\frac{1}{\epsilon^{2}}} \left(\frac{1}{\epsilon} \frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} (1+o(1)) \right) \int_{2}^{3} e^{-\frac{1}{\epsilon^{2}}} d\xi \\ &\leq \left(\frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} (1+o(1)) \right) \epsilon \\ &\longrightarrow 0. \end{split}$$

This proves the second part of (1.29).

5. Finally, if $\xi \in (-\delta, \delta)$, then we have $H(\xi) = 1 + \frac{H''(0)}{2}\xi^2(1 + O(|\xi|))$ by Taylor expansion, and therefore, similar to Step 2,

$$\begin{split} \int_{-\delta}^{\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi &= \frac{e^{-\frac{H_{\epsilon}}{\epsilon^{2}}}}{\epsilon^{2}} \int_{-\delta}^{\delta} e^{\frac{H''(0)}{2} \frac{\xi^{2}}{\epsilon^{2}} (1+O(|\xi|))} d\xi \\ &= \left(\frac{1}{\epsilon} \frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} (1+o(1))\right) \epsilon \int_{-\frac{\delta}{\epsilon}}^{\frac{\delta}{\epsilon}} e^{-\frac{|H''(0)|}{2} \xi^{2} (1+O(\epsilon|\xi|))} d\xi \\ &= \left(\frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} (1+o(1))\right) (1+o(1)) \int_{-\frac{\delta}{\epsilon}}^{\frac{\delta}{\epsilon}} e^{-\frac{|H''(0)|}{2} \xi^{2}} d\xi \\ &\longrightarrow \frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} \int_{-\infty}^{\infty} e^{-\frac{|H''(0)|}{2} \xi^{2}} d\xi \end{split}$$

$$= \frac{2\sqrt{2\pi}}{\sqrt{H''(1)}} \frac{\sqrt{2\pi}}{\sqrt{|H''(0)|}} \\ = \frac{4\pi}{\sqrt{|H''(0)| H''(1)}} \\ = \frac{2}{\kappa}.$$

We thereby obtain the second part of (1.30).

1.7 A compactness lemma

We are now ready to extract a convergent subsequence from ρ^{ϵ} . For this, let us first clarify the definition of weak- \star convergence that we will use.

Definition. Given a measurable subset X of \mathbb{R}^d , we say that a measure μ^{ϵ} on X converges weakly- \star to a measure μ , and we write $\mu^{\epsilon} \stackrel{\star}{\rightharpoonup} \mu$, if, for every $\phi \in C^0(\overline{X})$,

$$\int_{\overline{X}} \phi d\mu^{\epsilon} \longrightarrow \int_{\overline{X}} \phi d\mu.$$

Lemma 4. There exists a subsequence of ρ^{ϵ} (relabeled as ρ^{ϵ}) and functions $\alpha = \alpha(x, t)$ and $\beta = \beta(x, t)$, with $\alpha, \beta \in H^1(U \times [0, T])$, such that

1. ρ^{ϵ} is a probability measure on $D \times [0, T]$ that converges weakly- \star to $\alpha \delta_{-1} + \beta \delta_1$, such that, as $\epsilon \to 0$,

$$\int_{-1-\delta}^{-1+\delta} \rho^{\epsilon}(x,\xi,t)d\xi \rightharpoonup \alpha(x,t), \qquad \int_{1-\delta}^{1+\delta} \rho^{\epsilon}(x,\xi,t)d\xi \rightharpoonup \beta(x,t)$$
(1.31)

weakly in $L^2(U \times [0,T])$, and

$$\int_{\mathbb{R}\backslash I_{\delta}} \int_{U} |\rho^{\epsilon}(x,\xi,t)| \, dxd\xi \longrightarrow 0 \tag{1.32}$$

uniformly in $t \in [0, T]$.

2. ρ_t^{ϵ} is a measure on $D \times [0,T]$ that converges weakly- \star to $\alpha_t \delta_{-1} + \beta_t \delta_1$, such that, as $\epsilon \to 0$,

$$\int_{-1-\delta}^{-1+\delta} \rho_t^{\epsilon}(x,\xi,t)d\xi \rightharpoonup \alpha_t(x,t), \qquad \int_{1-\delta}^{1+\delta} \rho_t^{\epsilon}(x,\xi,t)d\xi \rightharpoonup \beta_t(x,t)$$
(1.33)

weakly in $L^2(U \times [0,T])$ and

$$\int_{\mathbb{R}\backslash I_{\delta}} \int_{U} |\rho_{t}^{\epsilon}(x,\xi,t)| \, dxd\xi \longrightarrow 0 \tag{1.34}$$

strongly in $L^2[0,T]$.

3. For every $i = 1 \cdots n$, $\rho_{x_i}^{\epsilon}$ (the *i*-th component of $\nabla \rho^{\epsilon}$) is a measure on $D \times [0, T]$ that converges weakly- \star to $\alpha_{x_i}\delta_{-1} + \beta_{x_i}\delta_1$, such that, as $\epsilon \to 0$,

$$\int_{-1-\delta}^{-1+\delta} \rho_{x_i}^{\epsilon}(x,\xi,t)d\xi \rightharpoonup \alpha_{x_i}(x,t), \qquad \int_{1-\delta}^{1+\delta} \rho_{x_i}^{\epsilon}(x,\xi,t)d\xi \rightharpoonup \beta_{x_i}(x,t)$$
(1.35)

weakly in $L^2(U \times [0,T])$, and

$$\int_{\mathbb{R}\backslash I_{\delta}} \int_{U} \left| \rho_{x_{i}}^{\epsilon}(x,\xi,t) \right| dxd\xi \longrightarrow 0$$
(1.36)

uniformly in $t \in [0, T]$.

Proof. 1. Writing $\rho^{\epsilon} = u^{\epsilon} \sigma^{\epsilon} = \left(\left(u^{\epsilon} \right)^2 \sigma^{\epsilon} \right)^{\frac{1}{2}} \cdot \left(\sigma^{\epsilon} \right)^{\frac{1}{2}}$, we get

$$\sup_{t \in [0,T]} \left(\int_{\mathbb{R} \setminus I_{\delta}} \int_{U} |\rho^{\epsilon}| \, dx d\xi \right)^{2} \leq t \in [0,T] \left(\int_{D} |u^{\epsilon}|^{2} \, \sigma^{\epsilon} dx d\xi \right) \left(\int_{\mathbb{R} \setminus I_{\delta}} \sigma^{\epsilon} d\xi \right) \longrightarrow 0.$$

This follows because the first term on the right is bounded by (1.18), whereas the second goes to 0 by the second part of (1.28). Therefore (1.32) follows.

In the same way, we get

$$\sup_{t \in [0,T]} \left(\int_{\mathbb{R} \setminus I_{\delta}} \int_{U} |\nabla \rho^{\epsilon}| \, dx d\xi \right)^{2} \leq t \in [0,T] \left(\int_{D} |\nabla u^{\epsilon}|^{2} \, \sigma^{\epsilon} dx d\xi \right) \left(\int_{\mathbb{R} \setminus I_{\delta}} \sigma^{\epsilon} d\xi \right) \longrightarrow 0,$$

and we deduce (1.36).

Finally, this time using (1.23) instead of (1.18), we get

$$\int_{0}^{T} \left(\int_{\mathbb{R} \setminus I_{\delta}} \int_{U} |\rho_{t}^{\epsilon}| \, dx d\xi \right)^{2} dt \leq \int_{0}^{T} \left(\int_{D} |u_{t}^{\epsilon}|^{2} \, \sigma^{\epsilon} dx d\xi \right) \left(\int_{\mathbb{R} \setminus I_{\delta}} \sigma^{\epsilon} d\xi \right) dt \longrightarrow 0,$$

and we obtain (1.34).

2. Define $\alpha^{\epsilon} = \alpha^{\epsilon}(x,t)$ and $\beta^{\epsilon} = \beta^{\epsilon}(x,t)$ as

$$\alpha^{\epsilon}(x,t) := \int_{-1-\delta}^{-1+\delta} \rho^{\epsilon}(x,\xi,t)d\xi = \int_{-1-\delta}^{-1+\delta} u^{\epsilon}(x,\xi,t)\sigma^{\epsilon}d\xi,$$
$$\beta^{\epsilon}(x,t) := \int_{1-\delta}^{1+\delta} \rho^{\epsilon}(x,\xi,t)d\xi = \int_{1-\delta}^{1+\delta} u^{\epsilon}(x,\xi,t)\sigma^{\epsilon}d\xi.$$

In the same way as above, but this time using the third part of (1.28), we obtain

$$\int_{0}^{T} \int_{U} |\alpha^{\epsilon}|^{2} dx dt \leq \int_{0}^{T} \left(\int_{-1-\delta}^{-1+\delta} \int_{U} |u^{\epsilon}|^{2} \sigma^{\epsilon} dx d\xi \right) \left(\int_{-1-\delta}^{-1+\delta} \sigma^{\epsilon} d\xi \right) dt \leq C,$$
$$\int_{0}^{T} \int_{U} |\alpha^{\epsilon}_{t}|^{2} dx dt \leq \int_{0}^{T} \left(\int_{-1-\alpha}^{-1+\alpha} \int_{U} |u^{\epsilon}_{t}|^{2} \sigma^{\epsilon} dx d\xi \right) \left(\int_{-1-\delta}^{-1+\delta} \sigma^{\epsilon} d\xi \right) dt \leq C,$$
$$\int_{0}^{T} \int_{U} |\nabla \alpha^{\epsilon}|^{2} dx dt \leq \int_{0}^{T} \left(\int_{-1-\delta}^{-1+\delta} \int_{U} |\nabla u^{\epsilon}|^{2} \sigma^{\epsilon} dx d\xi \right) \left(\int_{-1-\delta}^{-1+\delta} \sigma^{\epsilon} d\xi \right) dt \leq C.$$

The argument for β^{ϵ} is identical, and therefore $\{\alpha^{\epsilon}\}_{\epsilon>0}$ and $\{\beta^{\epsilon}\}_{\epsilon>0}$ are bounded in $H^1(U \times [0,T])$, a reflexive Banach space, and so, by weak compactness, we can extract a subsequence (not relabeled), such that, for some limit functions $\alpha = \alpha(x,t), \beta = \beta(x,t)$,

$$\alpha^{\epsilon}, \beta^{\epsilon} \rightharpoonup \alpha, \beta$$
 weakly in $H^1(U \times [0, T])$ as $\epsilon \to 0$.

(1.31), (1.33), and (1.35) then follow by construction.

From now on, we will chose the subsequence as above. This entails no loss of generality because, since the limits α and β are unique, the main result below will hold for all subsequences.

The following lemma, pointwise in nature, concerns the convergence of u^{ϵ} and its relationship with α and β .

Lemma 5. For every $t \in [0,T]$, as $\epsilon \to 0$, we have

$$\begin{cases} u^{\epsilon} \to 2\alpha & a.e. \ on \ U \times (-2,0) \\ u^{\epsilon} \to 2\beta & a.e. \ on \ U \times (0,2). \end{cases}$$

Proof. For every a and b fixed such that -2 < a < b < 0,

$$\begin{split} \int_{a}^{b} \int_{U} \left| u_{\xi}^{\epsilon} \right| dx d\xi &\leq \left(\int_{a}^{b} \int_{U} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u_{\xi}^{\epsilon} \right|^{2} dx d\xi \right)^{\frac{1}{2}} \left(\int_{a}^{b} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \right)^{\frac{1}{2}} \\ &\leq C \left(\int_{a}^{b} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \right)^{\frac{1}{2}} \quad (by \ (1.18)) \\ &\longrightarrow 0 \qquad (by \ (1.30)). \end{split}$$

Therefore, on $U \times [a, b]$, $u^{\epsilon} \longrightarrow u$ a.e. for some function u = u(x, t), and since a and b were arbitrary, this holds on $U \times (-2, 0)$. But using $\rho^{\epsilon} = \sigma^{\epsilon} u^{\epsilon}$, integrating with respect to ξ on $(-1 - \delta, -1 + \delta)$, and using (1.28) and (1.31), we get $u = 2\alpha$. The $U \times (0, 2)$ -case follows similarly.

Remark 1: The above proof shows that for a.e. x, the oscillation of $\xi \mapsto u^{\epsilon}(x,\xi,t)$ on [a,b] goes to 0. Therefore, without loss of generality, we can assume that the convergence holds a.e. on $U \times \{\xi = \pm \frac{3}{2}\}$.

Remark 2: Assumption (1.39) below asserts that the same result holds for t = 0 and $\xi = \pm \frac{3}{2}$.

1.8 Main theorem

We are now ready to state and prove our main theorem.

Theorem 2. Let u^{ϵ} be a solution to (1.4). Assume that the initial condition u_0^{ϵ} satisfies

$$\frac{1}{2} \int_{D} \sigma^{\epsilon} \left| u_{0}^{\epsilon} \right|^{2} dx d\xi \leq C, \tag{1.37}$$

$$\frac{1}{2} \int_{D} \sigma^{\epsilon} a^{\epsilon} \left| \nabla u_{0}^{\epsilon} \right|^{2} + \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| \partial_{\xi} u_{0}^{\epsilon} \right|^{2} dx d\xi \le C, \tag{1.38}$$

$$\begin{cases} u_0^{\epsilon} \to 2\alpha_0 & a.e. \text{ on } U \times \left\{ \xi = -\frac{3}{2} \right\} \\ u_0^{\epsilon} \to 2\beta_0 & a.e. \text{ on } U \times \left\{ \xi = \frac{3}{2} \right\}, \end{cases}$$
(1.39)

for some smooth $\alpha_0 = \alpha_0(x)$ and $\beta_0 = \beta_0(x)$, and where C is a constant independent of ϵ .

Moreover, assume that the diffusion coefficient a^{ϵ} satisfies

$$\sup_{\xi \in \mathbb{R}} |a^{\epsilon}(\xi)| \le C, \tag{1.40}$$

$$a^{\epsilon} \to a = a(\xi) \text{ uniformly on } \left(-\frac{3}{2}, -\frac{1}{2}\right) \text{ and } \left(\frac{1}{2}, \frac{3}{2}\right),$$
 (1.41)

where C is a (possibly different) constant independent of ϵ and ξ .

Then, on $D \times [0,T]$, as $\epsilon \to 0$, we have

$$\rho^{\epsilon}(x,\xi,t) \stackrel{\star}{\rightharpoonup} \alpha(x,t)\delta_{-1} + \beta(x,t)\delta_{1},$$

where the functions $\alpha = \alpha(x,t)$ and $\beta = \beta(x,t)$ are weak solutions of the following system of **reaction-diffusion** equations:

$$\begin{cases} \alpha_t - a_{-1}\Delta\alpha = \kappa (\beta - \alpha) & in U \times [0, T] \\ \beta_t - a_1 \Delta\beta = \kappa (\alpha - \beta) \\ \frac{\partial \alpha}{\partial \nu} = \frac{\partial \beta}{\partial \nu} = 0 & on \partial U \times [0, T] \\ \alpha = \alpha_0, \beta = \beta_0 & on U \times \{t = 0\}. \end{cases}$$
(1.42)

1.9 Proof of the main theorem

As mentioned above, here we provide a direct proof, using a cutoff function ψ and a cleverly designed test-functions $\phi^{1,\epsilon}$ and $\phi^{2,\epsilon}$ which cancel out the $\sigma^{\epsilon}/\tau_{\epsilon}$ -term in (1.4).

Proof. 1. Let $\psi = \psi(\xi) \in [0, 1]$ be a smooth and even cutoff-function, supported on [-3, 3], with $\psi \equiv 1$ on $\left[-\frac{5}{2}, \frac{5}{2}\right]$ and $|\psi'| \leq C$ for some positive constant C independent of ξ .



Figure 1.5: The cutoff function ψ

Define the test function

$$\phi^{1,\epsilon}(\xi) := \int_0^{b^{1}(\xi)} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi,$$

where

$$b^{1}(\xi) := \begin{cases} -\frac{3}{2} & \text{if } \xi < -\frac{3}{2} \\ \xi & \text{if } -\frac{3}{2} < \xi < \frac{3}{2} \\ \frac{3}{2} & \text{if } \xi > \frac{3}{2}, \end{cases}$$



Figure 1.6: The functions b^1 and b^2

and finally, let $\zeta = \zeta(x,t) \in C_c^{\infty}(U \times [0,T])$ be arbitrary.

Multiplying (1.4) by $\psi \phi^{1,\epsilon} \zeta$, integrating on $D \times [0,T]$ and recalling that $Supp(\psi) \subseteq [-3,3]$, we obtain

$$\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi - \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta a^{\epsilon} \left(\Delta u^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi = \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} \, dx dt d\xi, \quad (1.43)$$

and it remains to study all three terms of above identity.

2. Study of the first term on the left-hand-side of (1.43)

Write $u_t^{\epsilon} \sigma^{\epsilon} = \rho_t^{\epsilon}$ and split the first term up into three pieces to get

$$\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} dx dt d\xi = \int_{\mathbb{R} \setminus I_{\delta}} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \rho_{t}^{\epsilon} dx dt d\xi + \int_{-1-\delta}^{-1+\delta} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \rho_{t}^{\epsilon} dx dt d\xi + \int_{1-\delta}^{1+\delta} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \rho_{t}^{\epsilon} dx dt d\xi$$

$$(1.44)$$

Notice that $\phi^{1,\epsilon}$ is nondecreasing because $\tau_{\epsilon}/\sigma^{\epsilon} \geq 0$ and because $b^{1,\epsilon}$ is nondecreasing. Therefore, on $\left(-\frac{3}{2}, \frac{3}{2}\right)$, $\phi^{1,\epsilon}\left(-\frac{3}{2}\right) \leq \phi^{1,\epsilon}(\xi) \leq \phi^{1,\epsilon}\left(\frac{3}{2}\right)$, and in fact this is true for all $\xi \in \mathbb{R}$ because $\phi^{1,\epsilon}$ is continuous at $\xi = \pm \frac{3}{2}$ and constant on $\left(-\infty, -\frac{3}{2}\right)$ and $\left(\frac{3}{2}, \infty\right)$. But by (1.29) and (1.30), $\phi^{1,\epsilon}\left(\pm \frac{3}{2}\right) \rightarrow \pm \frac{1}{\kappa}$ as $\epsilon \rightarrow 0$. Therefore, for small ϵ , $\phi^{1,\epsilon}$ is uniformly bounded, i.e. there exists a constant C > 0, independent of ϵ , such that $|\phi^{1,\epsilon}| < C$.

Hence we can estimate

$$\left| \int_{\mathbb{R}\backslash I_{\delta}} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \rho_{t}^{\epsilon} \, dx dt d\xi \right| \leq \int_{\mathbb{R}\backslash I_{\delta}} \int_{0}^{T} \int_{U} |\psi| \left| \phi^{1,\epsilon} \right| \left| \zeta \right| \left| \rho_{t}^{\epsilon} \right| \, dx dt d\xi$$
$$\leq C \int_{0}^{T} \int_{\mathbb{R}\backslash I_{\delta}} \int_{U} \left| \rho_{t}^{\epsilon} \right| \, dx d\xi dt$$

$$\leq CT^{\frac{1}{2}} \left(\int_{0}^{T} \left(\int_{\mathbb{R} \setminus I_{\delta}} \int_{U} |\rho_{t}^{\epsilon}| \, dxd\xi \right)^{2} dt \right)^{\frac{1}{2}} \\ \longrightarrow 0 \qquad (by \ (1.32)).$$

Now because $\psi \equiv 1$ on $(\pm 1 - \delta, \pm 1 + \delta)$ for small δ , the other two integrals in (1.44) become

$$\int_{0}^{T} \int_{U} \left(\int_{\pm 1-\delta}^{\pm 1+\delta} \phi^{1,\epsilon} \rho_{t}^{\epsilon} d\xi \right) \zeta dx dt.$$
(1.45)

We isolate the convergence result for (1.45) in the following lemma:

Lemma 6.

$$\int_{0}^{T} \int_{U} \left(\int_{-1-\delta}^{-1+\delta} \phi^{1,\epsilon} \rho_{t}^{\epsilon} d\xi \right) \zeta dx dt \longrightarrow \left(-\frac{1}{\kappa} \right) \int_{0}^{T} \int_{U} \alpha_{t} \zeta dx dt,$$
$$\int_{0}^{T} \int_{U} \left(\int_{1-\delta}^{1+\delta} \phi^{1,\epsilon} \rho_{t}^{\epsilon} d\xi \right) \zeta dx dt \longrightarrow \frac{1}{\kappa} \int_{0}^{T} \int_{U} \beta_{t} \zeta dx dt.$$

Proof. We will only prove the second limit, as the first one is similar. Write

$$\int_{0}^{T} \int_{U} \left(\int_{1-\delta}^{1+\delta} \phi^{t} d\xi \right) \zeta dx dt - \frac{1}{\kappa} \int_{0}^{T} \int_{U} \beta_{t} \zeta dx dt = \int_{0}^{T} \int_{U} \int_{1-\delta}^{1+\delta} \left(\phi^{1,\epsilon} - \frac{1}{\kappa} \right) \rho_{t}^{\epsilon} \zeta d\xi dx dt + \frac{1}{\kappa} \int_{0}^{T} \int_{U} \left(\int_{1-\delta}^{1+\delta} (\rho_{t}^{\epsilon} - \beta_{t}) d\xi \right) \zeta dx dt.$$
(1.46)

The second term on the right-hand-side of (1.46) goes to 0 by (1.33) and the definition of weak convergence in $L^2(U \times [0, T])$. As for the first term, estimate it by

$$\begin{split} & \left| \int_0^T \int_U \int_{1-\delta}^{1+\delta} \left(\phi^{1,\epsilon} - \frac{1}{\kappa} \right) \rho_t^{\epsilon} \zeta d\xi dx dt \right| \\ \leq & \int_0^T \int_U \int_{1-\delta}^{1+\delta} \left| \phi^{1,\epsilon} - \frac{1}{\kappa} \right| \left| \rho_t^{\epsilon} \right| \left| \zeta \right| d\xi dx dt \\ \leq & C \left(\sup_{(1-\delta, 1+\delta)} \left| \phi^{1,\epsilon} - \frac{1}{\kappa} \right| \right) \int_0^T \int_U \int_{1-\delta}^{1+\delta} \left| \rho_t^{\epsilon} \right| d\xi dx dt \\ = & C \left(\sup_{(1-\delta, 1+\delta)} \left| \phi^{1,\epsilon} - \frac{1}{\kappa} \right| \right) \int_0^T \int_U \int_{1-\delta}^{1+\delta} \left| u_t^{\epsilon} \right| \sigma^{\epsilon} d\xi dx dt \end{split}$$

$$\leq C \left(\sup_{(1-\delta,1+\delta)} \left| \phi^{1,\epsilon} - \frac{1}{\kappa} \right| \right) \left(\int_{0}^{T} \int_{U} \int_{1-\delta}^{1+\delta} \sigma^{\epsilon} \left| u_{t}^{\epsilon} \right|^{2} d\xi dx dt \right)^{\frac{1}{2}} \left(\int_{0}^{T} \int_{U} \int_{1-\delta}^{1+\delta} \sigma^{\epsilon} d\xi dx dt \right)^{\frac{1}{2}} \\ = CT^{\frac{1}{2}} \left| U \right|^{\frac{1}{2}} \left(\sup_{(1-\delta,1+\delta)} \left| \phi^{1,\epsilon} - \frac{1}{\kappa} \right| \right) \left(\int_{0}^{T} \int_{U} \int_{1-\delta}^{1+\delta} \sigma^{\epsilon} \left| u_{t}^{\epsilon} \right|^{2} d\xi dx dt \right)^{\frac{1}{2}} \left(\int_{1-\delta}^{1+\delta} \sigma^{\epsilon} d\xi \right)^{\frac{1}{2}} \\ \leq C \left(\sup_{(1-\delta,1+\delta)} \left| \phi^{1,\epsilon} - \frac{1}{\kappa} \right| \right) \quad (by \ (1.23) \ \text{and} \ (1.28)).$$

However, because $\phi^{1,\epsilon}$ converges to $\frac{1}{\kappa}$ uniformly on $(1 - \delta, 1 + \delta)$ by (1.30), the last term above goes to 0 as $\epsilon \to 0$ as well, which concludes the proof.

It follows from Lemma 6 and (1.44) that

$$\lim_{\epsilon \to 0} \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi = \frac{1}{\kappa} \int_{0}^{T} \int_{U} \left(-\alpha_{t} + \beta_{t} \right) \zeta dx dt$$

3. Study of the second term on the left of (1.43)

Integrating by parts with respect to x and using $\frac{\partial u^{\epsilon}}{\partial \nu} = 0$ on $\partial U \times \mathbb{R} \times [0, T]$, we get

$$-\int_{-3}^{3}\int_{0}^{T}\int_{U}\psi\phi^{1,\epsilon}\zeta a^{\epsilon}\left(\Delta u^{\epsilon}\right)\sigma^{\epsilon}\,dxdtd\xi = \int_{-3}^{3}\int_{0}^{T}\int_{U}\psi\phi^{1,\epsilon}a^{\epsilon}\left(\nabla\zeta\right)\cdot\left(\nabla u^{\epsilon}\right)\sigma^{\epsilon}dxdtd\xi.$$
 (1.47)

Then, as before, split the right-hand-side of (1.47) up as

$$\int_{\mathbb{R}\backslash I_{\delta}} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} a^{\epsilon} (\nabla \zeta) \cdot (\nabla \rho^{\epsilon}) \, dx dt d\xi \\
+ \int_{-1-\delta}^{-1+\delta} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} a^{\epsilon} (\nabla \zeta) \cdot (\nabla \rho^{\epsilon}) \, dx dt d\xi + \int_{1-\delta}^{1+\delta} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} a^{\epsilon} (\nabla \zeta) \cdot (\nabla \rho^{\epsilon}) \, dx dt d\xi. \quad (1.48)$$

Using $|\psi| \leq 1, |\phi^{1,\epsilon}| \leq C, |\nabla \zeta| \leq C$, and now $|a^{\epsilon}| \leq C$ by (1.40), the first term in (1.48) is estimated by

$$\left| \int_{\mathbb{R}\backslash I_{\delta}} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} a^{\epsilon} \left(\nabla \zeta \right) \cdot \left(\nabla \rho^{\epsilon} \right) dx dt d\xi \right| \leq C \int_{0}^{T} \int_{\mathbb{R}\backslash I_{\delta}} \int_{U} \left| \nabla \rho^{\epsilon} \right| dx d\xi dt \longrightarrow 0 \quad (by \ (1.36)).$$

•

Because $\psi \equiv 1$ on $(\pm 1 - \delta, \pm 1 + \delta)$, the second and third term in (1.48) just become

$$\begin{split} &\int_0^T \int_U \left(\int_{-1-\delta}^{-1+\delta} \phi^{1,\epsilon} a^\epsilon \left(\nabla \rho^\epsilon \right) d\xi \right) \cdot \left(\nabla \zeta \right) dx dt, \\ &\int_0^T \int_U \left(\int_{1-\delta}^{1+\delta} \phi^{1,\epsilon} a^\epsilon \left(\nabla \rho^\epsilon \right) d\xi \right) \cdot \left(\nabla \zeta \right) dx dt. \end{split}$$

By Lemma 4, we know that for every i, $\rho_{x_i}^{\epsilon}$ weakly— \star converges to $(\alpha_{x_i}) \delta_{-1} + (\beta_{x_i}) \delta_1$ on $D \times [0, T]$. Moreover, by (1.29) and (1.30), $\phi^{1,\epsilon}$ converges uniformly to $-\frac{1}{\kappa}$ on $\left(-\frac{3}{2}, -\frac{1}{2}\right)$ and to $\frac{1}{\kappa}$ on $\left(\frac{1}{2}, \frac{3}{2}\right)$, and by (1.41) a^{ϵ} converges uniformly to a on those intervals, so by an adaptation of Lemma 6 to $\nabla \rho^{\epsilon}$, we conclude that

$$\int_0^T \int_U \left(\int_{-1-\delta}^{-1+\delta} \phi^{1,\epsilon} a^\epsilon \left(\nabla \rho^\epsilon \right) d\xi \right) \cdot \left(\nabla \zeta \right) dx dt \longrightarrow \int_0^T \int_U \left(-\frac{1}{\kappa} \right) a_{-1} \left(\nabla \alpha \right) \cdot \left(\nabla \zeta \right) dx dt,$$

$$\int_0^T \int_U \left(\int_{1-\delta}^{1+\delta} \phi^{1,\epsilon} a^\epsilon \left(\nabla \rho^\epsilon \right) d\xi \right) \cdot \left(\nabla \zeta \right) dx dt \longrightarrow \int_0^T \int_U \left(\frac{1}{\kappa} \right) a_1 \left(\nabla \beta \right) \cdot \left(\nabla \zeta \right) dx dt$$

It follows from this and (1.47) - (1.48) that

$$\lim_{\epsilon \to 0} -\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \left(\Delta \rho^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi = \frac{1}{\kappa} \int_{0}^{T} \int_{U} \left(-a_{-1} \nabla \alpha + a_{1} \nabla \beta \right) \cdot \left(\nabla \zeta \right) dx dt.$$

4. Study of the term on the right-hand-side of (1.43)

Integrating by parts with respect to ξ and using $\psi(\pm 3) = 0$, we obtain

$$\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} dx dt d\xi = -\int_{-3}^{3} \int_{0}^{T} \int_{U} \left(\psi \phi^{1,\epsilon} \right)_{\xi} \zeta \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} dx dt d\xi$$
$$= -\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi_{\xi} \phi^{1,\epsilon} \zeta \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} dx dt d\xi - \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi_{\xi}^{1,\epsilon} \zeta \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} dx dt d\xi \quad (1.49)$$

For the first integral on the right-hand-side of (1.49), recall that $|\psi_{\xi}| = |\psi'| \leq C$, $|\phi^{1,\epsilon}| \leq \frac{1}{\kappa}, |\zeta| \leq C$, and $\psi_{\xi} \equiv 0$ on $\left(-\frac{5}{2}, \frac{5}{2}\right)$. Therefore

$$\begin{split} \left| \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi_{\xi} \phi^{1,\epsilon} \zeta \; \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \, dx dt d\xi \right| &\leq \int_{-3}^{3} \int_{0}^{T} \int_{U} |\psi_{\xi}| \left| \phi^{1,\epsilon} \right| \left| \zeta \right| \; \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \left| u_{\xi}^{\epsilon} \right| \; dx dt d\xi \\ &\leq C \; \left(\int_{0}^{T} \int_{U} \int_{\mathbb{R}} \left| u_{\xi}^{\epsilon} \right|^{2} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \; dx dt d\xi \right)^{\frac{1}{2}} \left(\int_{\frac{5}{2}}^{3} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} d\xi \right)^{\frac{1}{2}} \\ &\leq C \left(\int_{\frac{5}{2}}^{3} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} d\xi \right)^{\frac{1}{2}} \; (by \; (1.23)) \\ &\longrightarrow 0 \quad (by \; (1.29)). \end{split}$$

As for the second integral on the right-hand-side of (1.49), by construction

$$\phi_{\xi}^{1,\epsilon} = \begin{cases} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} \text{ if } -\frac{3}{2} < \xi < \frac{3}{2} \\ 0 \quad \text{if } |\xi| > \frac{3}{2}, \end{cases}$$

and thus

$$-\int_{-3}^{3}\int_{0}^{T}\int_{U}\psi\phi_{\xi}^{1,\epsilon}\zeta\frac{\sigma^{\epsilon}}{\tau_{\epsilon}}u_{\xi}^{\epsilon}\,dxdtd\xi = -\int_{-\frac{3}{2}}^{\frac{3}{2}}\int_{0}^{T}\int_{U}\psi\zeta\frac{\tau_{\epsilon}}{\sigma^{\epsilon}}\frac{\sigma^{\epsilon}}{\tau_{\epsilon}}u_{\xi}^{\epsilon}\,dxdtd\xi$$
$$= -\int_{-\frac{3}{2}}^{\frac{3}{2}}\int_{0}^{T}\int_{U}\zeta\,u_{\xi}^{\epsilon}\,dxdtd\xi$$
$$(\text{because }\psi\equiv1\text{ on }(-3/2,3/2))$$
$$= \int_{0}^{T}\int_{U}\zeta\,u^{\epsilon}\left(x,t,-\frac{3}{2}\right) - \zeta\,u^{\epsilon}\left(x,t,\frac{3}{2}\right)\,dxdt$$
$$\longrightarrow \int_{0}^{T}\int_{U}\zeta\,(2\alpha-2\beta)\,dxdt \quad (\text{by Lemma 5}).$$

Combining (1.50) - (1.51) with (1.49), we get

$$\lim_{\epsilon \to 0} \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} \, dx dt d\xi = \int_{0}^{T} \int_{U} \zeta \left(2\alpha - 2\beta \right) dx dt.$$

5. To conclude, letting $\epsilon \to 0$ in (1.43) and using Steps 2 – 4, we to deduce that α and β must satisfy

$$\frac{1}{\kappa} \int_0^T \int_U \left(-\alpha_t + \beta_t\right) \zeta dx dt + \frac{1}{\kappa} \int_0^T \int_U \left(-a_{-1} \nabla \alpha + a_1 \nabla \beta\right) \cdot \left(\nabla \zeta\right) dx dt$$
$$= \int_0^T \int_U \zeta \left(2\alpha - 2\beta\right) dx dt. \quad (1.52)$$

Approximating general $\zeta \in H_0^1(U \times [0,T])$ with $\zeta \in C_c^{\infty}(U \times [0,T])$, we conclude that (1.52) holds for $\zeta \in H_0^1(U \times [0,T])$ as well, and therefore α and β are weak solutions of

$$\frac{1}{\kappa} \left(-\alpha_t + \beta_t \right) + \frac{1}{\kappa} \left(a_{-1} \Delta \alpha - a_1 \Delta \beta \right) = 2\alpha - 2\beta,$$

which we can rewrite as

$$(\alpha_t - \beta_t) + (-a_{-1}\Delta\alpha + a_1\Delta\beta) = 2\kappa \left(\beta - \alpha\right).$$
(1.53)

6. We need another identity relating α and β . For this, repeat the same proof as above, but this time define

$$\phi^{2,\epsilon}(\xi) := \int_0^{b^2(\xi)} \frac{\tau_\epsilon}{\sigma^\epsilon} d\xi,$$

where (see again Figure 1.6)

$$b^{2}(\xi) := \begin{cases} -\frac{3}{2} & \text{if } \xi < -\frac{3}{2} \\ \xi & \text{if } -\frac{3}{2} < \xi < -\frac{1}{2} \\ -\frac{1}{2} & \text{if } \xi > -\frac{1}{2}. \end{cases}$$

Using $\psi \phi^{2,\epsilon} \zeta$ as our new test-function in (1.4), and integrating on $D \times [0,T]$, we get

$$\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{2,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi - \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{2,\epsilon} \zeta a^{\epsilon} \left(\Delta u^{\epsilon}\right) \sigma^{\epsilon} \, dx dt d\xi = \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{2,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon}\right)_{\xi} \, dx dt d\xi. \quad (1.54)$$

As before, because $\phi^{2,\epsilon}(\xi)$ converges uniformly to $-\frac{1}{\kappa}$ on $\left(-\frac{3}{2}, -\frac{1}{2}\right)$ and to $-\frac{1}{\kappa}$ on $\left(\frac{1}{2}, \frac{3}{2}\right)$, the first integral on the left-hand-side of (1.54) converges to

$$\lim_{\epsilon \to 0} \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{2,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} d\xi dx dt = -\frac{1}{\kappa} \int_{0}^{T} \int_{U} (\alpha_{t} + \beta_{t}) \zeta dx dt.$$

By the same argument, the second integral on the left-hand-side of (1.54) converges to
$$\lim_{\epsilon \to 0} \int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{2,\epsilon} \left(\nabla \rho^{\epsilon} \right) \cdot \left(\nabla \zeta \right) \, d\xi dx dt = -\frac{1}{\kappa} \int_{0}^{T} \int_{U} \left(\nabla \alpha + \nabla \beta \right) \cdot \nabla \zeta dx dt.$$

Finally, integrating the right-hand-side of (1.54) by parts with respect to ξ , and using that

$$\phi_{\xi}^{2,\epsilon} = \begin{cases} 0 & \text{if } \xi < -\frac{3}{2} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } -\frac{3}{2} < \xi < -\frac{1}{2} \\ 0 & \text{if } \xi > -\frac{1}{2}, \end{cases}$$

we see that the right-hand-side of (1.54) converges to

$$\lim_{\epsilon \to 0} -\int_{-3}^{3} \int_{0}^{T} \int_{U} \psi \phi^{2,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} dx dt d\xi = \int_{0}^{T} \int_{U} \zeta \left(2\alpha - 2\alpha \right) dx dt = 0.$$

By (1.54) and an approximation-argument, we deduce that α and β are weak solutions of

$$\frac{1}{\kappa} \left(-\alpha_t - \beta_t \right) + \frac{1}{\kappa} \left(a_{-1} \Delta \alpha + a_1 \Delta \beta \right) = 0,$$

which can be rewritten as

$$\alpha_t + \beta_t - (a_{-1}\Delta\alpha + a_1\Delta\beta) = 0. \tag{1.55}$$

7. In conclusion, putting (1.53) and (1.55) together, we get that α and β are weak solutions to

$$\begin{cases} \alpha_t - \beta_t + (-a_{-1}\Delta\alpha + a_1\Delta\beta) &= 2\kappa \left(\beta - \alpha\right) \\ \alpha_t + \beta_t + (-a_{-1}\Delta\alpha - a_1\Delta\beta) &= 0, \end{cases}$$

which, solving for α_t and β_t , gives the desired reaction-diffusion system

$$\begin{cases} \alpha_t - a_{-1}\Delta\alpha = \kappa(\beta - \alpha) \\ \beta_t - a_1\Delta\beta = \kappa(\alpha - \beta). \end{cases}$$
(1.56)

8. Initial Condition

By comparing assumption (1.39) and Lemma 5 with t = 0 and $\xi = \pm \frac{3}{2}$, we obtain that $\alpha(x, 0) = \alpha_0(x)$ and $\beta(x, 0) = \beta_0(x)$.

9. Boundary condition

First of all, notice that, in the above proof, we have never used the fact that ζ vanishes on $\partial U \times [0, T]$. Therefore, we can repeat the same proof, this time assuming $\zeta \in C^{\infty}(\overline{U} \times [0, T])$

only, and hence, by approximation, we deduce that (1.52) is valid for all $\zeta \in H^1(\overline{U} \times [0,T])$. Moreover, regularity theory for linear constant-coefficient systems of parabolic PDE implies that α and β are in fact smooth. This allows us to integrate by parts with respect to x in the second term on the left-hand-side of (1.52) again to obtain

$$\begin{aligned} \frac{1}{\kappa} \int_0^T \int_U \left(-\alpha_t + \beta_t \right) \zeta dx dt &+ \frac{1}{\kappa} \int_0^T \int_{\partial U} \left(-a_{-1} \frac{\partial \alpha}{\partial \nu} + a_1 \frac{\partial \beta}{\partial \nu} \right) \zeta dx dt \\ &+ \frac{1}{\kappa} \int_0^T \int_{\partial U} \left(a_{-1} \Delta \alpha - a_1 \Delta \beta \right) \zeta dx dt = \int_0^T \int_U \left(2\alpha - 2\beta \right) \zeta dx dt, \end{aligned}$$

which we may rewrite as

$$\frac{1}{\kappa} \int_0^T \int_{\partial U} \left(-a_{-1} \frac{\partial \alpha}{\partial \nu} + a_1 \frac{\partial \beta}{\partial \nu} \right) \zeta dx dt = \frac{1}{\kappa} \int_0^T \int_U \left(\alpha_t - \beta_t - a_{-1} \Delta \alpha + a_1 \Delta \beta + 2\kappa \alpha - 2\kappa \beta \right) \zeta dx dt.$$
(1.57)

However, because α and β are smooth, it follows from (1.56) that the right-hand-side of (1.57) is 0, and therefore

$$\int_{0}^{T} \int_{\partial U} \left(-a_{-1} \frac{\partial \alpha}{\partial \nu} + a_{1} \frac{\partial \beta}{\partial \nu} \right) \zeta dx dt = 0.$$

Since ζ was arbitrary in $H^1(U \times [0, T])$, we get that

$$-a_{-1}\frac{\partial\alpha}{\partial\nu} + a_1\frac{\partial\beta}{\partial\nu} = 0 \tag{1.58}$$

in the weak sense on $\partial U \times [0, T]$.

Likewise, using the integrated version of (1.55), one obtains that

$$-a_{-1}\frac{\partial\alpha}{\partial\nu} - a_1\frac{\partial\beta}{\partial\nu} = 0.$$
(1.59)

in the weak sense. Solving for $\frac{\partial \alpha}{\partial \nu}$ and $\frac{\partial \beta}{\partial \nu}$ in (1.58) and (1.59) we obtain that $\frac{\partial \alpha}{\partial \nu} = 0$ and $\frac{\partial \beta}{\partial \nu} = 0$ in the weak sense. But by (1.42) and again by the regularity theory for linear constant-coefficient systems of parabolic PDE, this holds in the classical sense as well.

1.10 Comparison with other methods of proof

As mentioned before, the convergence result in the main theorem has already been proved independently by Peletier-Savaré-Veneroni [48], Herrmann-Niethammer [29], and Arnrich et. al. [3]. In this section, we briefly outline their proofs. Notice in particular the similarity in their approach: all three papers reformulate both (1.3) and (1.5) in a common variational framework; an L^2 gradient flow-structure for [48], and a Wasserstein structure for [29] and [3]. This is motivated by a recent trend to use gradient-flow structures to pass to the limit in general time-evolving systems; see for example the papers by Ambrosio et. al. [2], Mielke et. al. [41], Mielke and Stefanelli [42], Sandier [53], Serfaty [55], or Stefanelli [59]. Moreover, in order to pass to the limit they all use (a version of) Γ -convergence, which is one of the most powerful tools for the rigorous study of singular variational problems. See the papers by Dal Maso [17] and De Giorgi et. al. [18] for an overview of Γ -convergence.

Proof by Peletier-Savaré-Veneroni

The authors in [48] prove the same result as in the main theorem, but under slightly weaker assumptions; namely, they do not assume (1.38) any more, and (1.39) is replaced with an assumption on the weak- \star -convergence of ρ_0^{ϵ} . Moreover, their potential function H is only defined on [-1, 1], which leads to the following change in the definition of κ :

$$\kappa = \frac{\sqrt{|H''(0)| H''(1)}}{\pi}.$$

The main idea in their proof is to rewrite both (1.4) and (1.5) as variational evolution equations in a common space of measures. Inspired by the ideas of Spagnolo [57, 58, 20] (see also the books by Attouch [5] and Brézis [14]), they rewrite both equations as L^2 gradient flow structures. The advantage of this formulation is to shift the study of the convergence of solutions to the convergence of quadratic forms.

The second main idea is to pass to the limit in the formulation for (1.4). After stating and proving regularization estimates similar to (1.18) and (1.23), the authors then show that the quadratic forms associated to (1.4) Γ -converge to the ones associated to (1.5). This entails in proving both a liminf-inequality, as well as a limsup-property. Using this, one can finally pass to the limit as $\epsilon \to 0$ in the formulation of (1.4), to eventually obtain the formulation of (1.5).

In their proof, an important role is played by the minimal transition cost

$$K^{\epsilon}(\phi^{-},\phi^{+}) := \left\{ \tau_{\epsilon} \int_{-1}^{1} \left(\phi'(\xi) \right)^{2} \sigma^{\epsilon} d\xi : \phi \in H^{1}(-1,1), \phi(\pm 1) = \phi^{\pm} \right\}.$$

This can be used to construct an appropriate interpolation between the 'boundary values' ϕ^{\pm} . One can moreover show that

$$\lim_{\epsilon \to 0} K^{\epsilon} \left(-\frac{1}{2}, \frac{1}{2} \right) = \kappa.$$
(1.60)

This gives a new interpretation of the constant κ , which can now be seen as the limit of the minimal transition cost. Let us note that, in our forthcoming paper with Evans [21], we use an analog of K^{ϵ} to treat the higher-dimensional version of (1.3).

The authors also prove a slightly stronger convergence-result, which says that, under the additional assumption of 'strong' convergence of the initial data, we have an appropriate 'strong' convergence of the solutions (cf. the papers by Hutschinson [31] and Rešetnjak[51], as well as section 5.4 in Ambrosio et. al. [1]). This notion is inspired by Hilbert spaces, where strong convergence is equivalent to weak convergence together with convergence of the norms. The convergence here is strong enough to pass to the limit in suitable nonlinear functions of u^{ϵ} , cf. Corollary 3.3 in Peletier-Savaré-Veneroni [48].

Finally, let us remark that their proof relies heavily on the linearity of (1.4); for example they use the parallelogram law to extend the definitions of the quadratic forms. It is not clear to us how to adapt the proof to study nonlinear versions of (1.4).

Proof by Herrmann-Niethammer

The authors in [29] provide a different proof of the same result, in an attempt to answer the following question posed by Peletier-Savaré-Veneroni [48]: "Can (1.3) and (1.5) be interpreted within the Wasserstein gradient flow-framework?" This Wasserstein-structure was pioneered by Otto (see the papers by Otto et. al. [47] and Jordan et. al. [32]) and relies on the interpretation of ρ^{ϵ} as a mass distribution that is transported so as to reduce a certain free energy. This structure is known to arise in a wide range of models of systems; see for example the papers by Ambrosio [1], Blanchet et. al. [12], Carrillo et. al. [16], Gangbo et. al. [15], Gigli [25], Gianazza et. al. [24], Matthes et. al. [39], and Savaré [54].

The crux of their proof lies in expressing both (1.3) and (1.5) as integrated Rayleigh principles. This principle has previously only been used in finite dimensions (see for example the papers by Otto [46] and Niethammer-Oshita [45]), so the application to parabolic PDE is new. The rough idea is to interpret the solutions of (1.3) and (1.5) as minimizers of suitable integral energy functionals on manifolds. The authors then show that the Rayleigh principle associated to (1.4) Γ -converges to the one associated to (1.5), which, as usual, entails a liminf-inequality and a limsup-property (technically, they only show that the liminf-inequality only holds along a particular sequence of minimizers, but this is enough to conclude).

It is to be noted that their proof starts out identical to ours, in the sense that they prove the regularization estimates (1.18) and (1.23), and show that the compactness estimates (1.28) - (1.29) in Lemma 3 hold, thereby extracting suitable convergent subsequences of ρ^{ϵ} , as in Lemma 4. In addition, although they do not explicitly state it, they also use the Prahgmen-Lindelöf principle (Theorem 10 in section 2.6 of the book by Protter and Weinberger [49]), a version of the maximum principle that applies to unbounded domains, to show that we have $u^{\epsilon} > C$ for some constant C > 0 independent of ϵ . This is useful to estimate terms involving $1/u^{\epsilon}$.

An important tool in their proof is the following first-order approximation \tilde{u}^{ϵ} , of u^{ϵ} , which can be contrasted with Lemma 5:

$$\tilde{u}^{\epsilon}(x,t) := 1 + (u(t) - 1)\eta^{\epsilon}(x), \text{ where } \eta^{\epsilon}(x) := 2\left(\frac{\int_0^x 1/\sigma^{\epsilon} dy}{\int_{-1}^1 1/\sigma^{\epsilon} dy}\right).$$

It says that u^{ϵ} is close to a step-function, but exhibits a narrow boundary-layer near x = 0, whose shape is determined by σ^{ϵ} (here the authors use x instead of ξ), as depicted in Figure 1.7.



Figure 1.7: u^{ϵ} exhibiting a boundary layer at 0

Notice that by using our test functions $\phi^{1,\epsilon}$ and $\phi^{2,\epsilon}$, we effectively bypass this transition layer, as witnessed by the term $u^{\epsilon}(x, -\frac{3}{2}, t) - u^{\epsilon}(x, \frac{3}{2}, t)$ in (1.51).

Proof by Arnrich et. al.

According to the authors in [3], the main issue with the proof of Herrmann-Niethammer [29] is that the compactness results (Lemma 4) do not follow from the Wasserstein gradient structure, but instead from the L^2 gradient-flow structure; this is because Herrmann and Niethammer rely on the estimates (1.18) and (1.23) instead of estimates provided by the

Wasserstein-structure. Moreover, they note that the integrated Rayleigh-principle is generally ill-behaved with respect to perturbations of the minimizers. They provide an example of a functional I for which, given a certain minimizer u, there is a sequence of functions u^n converging to u for which the value of the integrated Rayleigh principle of I at u^n diverges to $-\infty$.

As a consequence, in their paper [3] (which can be considered as a sequel of the paper by Peletier-Savaré-Veneroni [48]), the authors try to correct those issues, and furthermore provide a complete answer to the question posed in the previous section. They solve the problem (with Robin boundary-conditions) using the Wasserstein gradient flow-structure of (1.3) only (see the papers by Otto [47], and Jordan [32]). To achieve this, they rewrite both (1.3) and (1.5) in the form $\mathcal{A}(z; 0, T) = 0$, where \mathcal{A} in the (1.3)-case is an action functional that captures the property of z being a curve of 'maximal slope,' and \mathcal{A} in the (1.5)-case is a "simplified" action functional. This formulation was pioneered by DeGiorgi (see De Giorgi et. al. [19]) and further studied in Sandier [53] and Stefanelli [59], and can be generalized to topological spaces equipped with a lower semicontinuous pseudo-distance. It is interesting to note that, for \mathcal{A} in (1.5), they use a similar minimal transition cost to interpolate between values of u at $\xi = \pm 1$.

Then, just like in the above papers, after proving a suitable compactness result for ρ^{ϵ} , they show that the formulation of (1.3) Γ -converges to the one of (1.5), which again involves a liminf-inequality and a limsup-property (although, strictly speaking, the latter property is not really needed). Their proof involves a mixture of measure theory, optimal transport and entropy-dissipation-techniques, and the use of certain continuity-equations (see the paper by Benamou-Brenier [6]). Interestingly, note that for the compactness result, one only needs the fact that $\mathcal{A}(\rho^{\epsilon})$ is uniformly bounded with respect to ϵ , which allows them to potentially generalize this result to a wider class of equations.

A second fundamental idea in their proof is a change of variable $\xi \mapsto s$, which changes the function u^{ϵ} , which has a near-discontinuity at $\xi = 0$, to a smooth function \hat{u}^{ϵ} that has a slope of order O(1), as in Figure 1.8 on the next page. This approach is reminiscent of the cell-problem in homogenization (see Hornung [30]) or the 'inner' and 'outer'-layers in singular perturbation theory (see Villani [60]). This change of variable allows the authors to desingularize the diffusion term $\tau_{\epsilon} u^{\epsilon}_{\xi\xi}$, and therefore enables them to study the limit behavior of u^{ϵ} more carefully.



Figure 1.8: The smoothing effect of the change of variable $\xi \mapsto s$ (adapted from Arnrich [3])

Chapter 2

A Triple Well-Model

2.1 Introduction

In this chapter, $H = H(\xi)$ is a smooth, nonnegative, and even triple-well potential function with H(1) = H(3) = 1, H(0) = H(2) = 0, local minima at 0 and 2, a local maximum at 1, and is increasing on (0, 1), decreasing on (1, 2), and increasing on $(2, \infty)$. Assume furthermore that H''(0) = H''(2); we will get rid of this last assumption in section 2.4.



Figure 2.1: A triple-well potential function H

Given that most of the proofs in the previous chapter remain unchanged, we will only state the main results with the appropriate modifications.

2.2 Estimates

Basic estimates

The basic estimates (1.18) and (1.23) stay the same, and we make the same assumptions (1.37) and (1.38) on the initial conditions as before.

Study of the density σ^{ϵ}

The asymptotics for $e^{-\frac{\tilde{H}\epsilon}{\epsilon^2}}$ change to

$$\begin{split} e^{-\frac{\bar{H}_{\epsilon}}{\epsilon^{2}}} &= \int_{\mathbb{R}} e^{-\frac{H(\xi)}{\epsilon^{2}}} d\xi \\ &= \int_{-\infty}^{-1} e^{-\frac{H(\xi)}{\epsilon^{2}}} d\xi + \int_{-1}^{1} e^{-\frac{H(\xi)}{\epsilon^{2}}} d\xi + \int_{1}^{\infty} e^{-\frac{H(\xi)}{\epsilon^{2}}} d\xi \\ &= \epsilon \sqrt{2\pi} \left(\frac{1}{\sqrt{H''(-2)}} + \frac{1}{\sqrt{H''(0)}} + \frac{1}{\sqrt{H''(2)}} \right) (1 + o(1)) \\ &= \epsilon \frac{3\sqrt{2\pi}}{\sqrt{H''(0)}} (1 + o(1)). \end{split}$$

In the first equality, we used our normalization condition $\int_{\mathbb{R}} \sigma^{\epsilon} d\xi = 1$, whereas in the third equality, we used Laplace's method (Theorem 1) and our assumption that H''(-2) = H''(0) = H''(2). Therefore

$$e^{\frac{\bar{H}_{\epsilon}}{\epsilon^2}} = \frac{1}{\epsilon} \frac{\sqrt{H''(0)}}{3\sqrt{2\pi}} (1+o(1)).$$

Because of this change, we need to appropriately modify the compactness estimates (Lemma 3). Recall that $\delta = \delta(\epsilon) = \epsilon^{\frac{3}{4}}$.

Lemma 7. Define $I_{\delta} := (-2 - \delta, -2 + \delta) \cup (-\delta, \delta) \cup (2 - \delta, 2 + \delta)$ and $J_{\delta} := (-3 - \delta, -3 + \delta) \cup (-1 - \delta, -1 + \delta) \cup (1 - \delta, 1 + \delta) \cup (3 - \delta, 3 + \delta)$. As $\epsilon \to 0$, we have

$$\sup_{\mathbb{R}\setminus I_{\delta}} \sigma^{\epsilon} \longrightarrow 0, \qquad \int_{\mathbb{R}\setminus I_{\delta}} \sigma^{\epsilon} d\xi \longrightarrow 0, \qquad \int_{\pm 2-\delta}^{\pm 2+\delta} \sigma^{\epsilon} d\xi \longrightarrow \frac{1}{3}, \qquad \int_{-\delta}^{\delta} \sigma^{\epsilon} d\xi \longrightarrow \frac{1}{3}, \quad (2.1)$$

$$\inf_{(-3,3)\backslash J_{\delta}} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \longrightarrow \infty, \qquad \int_{(3,4)} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} d\xi \longrightarrow 0, \qquad (2.2)$$

$$\int_{\pm 1-\delta}^{\pm 1+\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow \frac{3}{\kappa}, \qquad \int_{(-3,3)\backslash J_{\delta}} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow 0.$$
(2.3)

Compactness lemma

We can therefore extract a convergence subsequence of ρ^{ϵ} (relabeled as ρ^{ϵ}), as well as functions $\alpha, \beta, \gamma \in H^1(U \times [0, T])$ such that $\rho^{\epsilon} \rightharpoonup \alpha \delta_{-2} + \beta \delta_0 + \gamma \delta_2$ with (appropriately modified) estimates as in Lemma 4.

Lemma 8. As $\epsilon \to 0$, we get

$$\begin{cases} u^{\epsilon} \to 3\alpha & a.e. \ on \ U \times (-3, -1) \\ u^{\epsilon} \to 3\beta & a.e. \ on \ U \times (-1, 1) \\ u^{\epsilon} \to 3\gamma & a.e. \ on \ U \times (1, 3). \end{cases}$$

Note: Without loss of generality, assume that the convergence holds a.e. on $U \times \{\xi = \pm \frac{5}{2}, -\frac{1}{2}\}$.

2.3 Main theorem

Theorem 3. Under the same assumptions (1.37), (1.38), and (1.40), but changing (1.39) to

$$\begin{cases} u_0^{\epsilon} \to 3\alpha_0 \quad a.e. \text{ on } U \times \left\{ \xi = -\frac{5}{2} \right\} \\ u_0^{\epsilon} \to 3\beta_0 \quad a.e. \text{ on } U \times \left\{ \xi = -\frac{1}{2} \right\} \\ u_0^{\epsilon} \to 3\gamma_0 \quad a.e. \text{ on } U \times \left\{ \xi = \frac{1}{2} \right\}, \end{cases}$$
(2.4)

for some smooth $\alpha_0 = \alpha_0(x), \beta_0 = \beta_0(x)$, and $\gamma_0 = \gamma_0(x)$; as well as changing (1.41) to

$$a^{\epsilon} \longrightarrow a = a(\xi) \text{ uniformly on } \left(-\frac{5}{2}, -\frac{3}{2}\right), \left(-\frac{1}{2}, \frac{1}{2}\right) \text{ and } \left(\frac{3}{2}, \frac{5}{2}\right),$$
 (2.5)

we get that, on $D \times [0, T]$, as $\epsilon \to 0$,

$$\rho^{\epsilon}(x,\xi,t) \stackrel{\star}{\rightharpoonup} \alpha(x,t)\delta_{-2} + \beta(x,t)\delta_{0} + \gamma(x,t)\delta_{2},$$

where the functions α , β , γ are weak solutions of the following system of **reaction-diffusion** equations:

$$\begin{cases} \alpha_t - a_{-2}\Delta\alpha = \kappa (\beta - \alpha) \\ \beta_t - a_0\Delta\beta = \kappa (\alpha - 2\beta + \gamma) & in U \times [0, T] \\ \gamma_t - a_2\Delta\gamma = \kappa (\beta - \gamma) \\ \frac{\partial \alpha}{\partial \nu} = \frac{\partial \beta}{\partial \nu} = \frac{\partial \gamma}{\partial \nu} = 0 & on \partial U \times [0, T] \\ \alpha = \alpha_0, \beta = \beta_0, \gamma = \gamma_0 & on U \times \{t = 0\}. \end{cases}$$

$$(2.6)$$

Proof. Since the proof is similar to the one in chapter 1, we will only lay out the main steps.

1. Let $\psi = \psi(\xi)$ be a smooth, even cutoff-function supported on [-4, 4] such that $0 \le \psi \le 1, \ \psi \equiv 1$ on $\left[-\frac{7}{2}, \frac{7}{2}\right]$, and $|\psi'| \le C$, as in the following figure:



Figure 2.2: The cutoff function ψ

Also define

$$\phi^{1,\epsilon}(\xi) := \int_{-1}^{b^{1}(\xi)} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi,$$

where

$$b^{1}(\xi) := \begin{cases} -\frac{5}{2} & \text{if } \xi < -\frac{5}{2} \\ \xi & \text{if } -\frac{5}{2} < \xi < -\frac{1}{2} \\ -\frac{1}{2} & \text{if } \xi > -\frac{1}{2}, \end{cases}$$



Figure 2.3: The functions b^1 , b^2 , and b^3

and finally, let $\zeta = \zeta(x,t) \in C_c^{\infty}(U \times [0,T])$ be arbitrary.

Using $\psi \phi^{1,\epsilon} \zeta$ as our test-function in (1.4), and integrating over $D \times [0,T]$, we get

$$\int_{-4}^{4} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi - \int_{-4}^{4} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta a^{\epsilon} \left(\Delta u^{\epsilon}\right) \sigma^{\epsilon} \, dx dt d\xi = \int_{-4}^{4} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon}\right)_{\xi} \, dx dt d\xi, \quad (2.7)$$

and it remains to study all three terms of above identity.

CHAPTER 2. A TRIPLE WELL-MODEL

2. Study of the first term on the left-hand-side of (2.7)

Since $\phi^{1,\epsilon}(\xi)$ converges uniformly to $-\frac{3}{2\kappa}$ on $\left(-\frac{5}{2},-\frac{3}{2}\right)$, to $\frac{3}{2\kappa}$ on $\left(-\frac{1}{2},\frac{1}{2}\right)$, and to $\frac{3}{2\kappa}$ on $\left(\frac{3}{2},\frac{5}{2}\right)$, the first term on the left-hand-side of (2.7) goes to

$$\lim_{\epsilon \to 0} \int_{-4}^{4} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi = \frac{3}{2\kappa} \int_{0}^{T} \int_{U} \left(-\alpha_{t} + \beta_{t} + \gamma_{t} \right) \zeta dx dt.$$
(2.8)

3. Study of the second term on the left-hand-side of (2.7)

Similarly, by (2.5), the second term on the left-hand-side of (2.7) goes to

$$\lim_{\epsilon \to 0} -\int_{-4}^{4} \int_{0}^{T} \int_{U} \psi \phi^{1,\epsilon} \zeta \left(\Delta u^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi = \frac{3}{2\kappa} \int_{0}^{T} \int_{U} \left(-a_{-2} \nabla \alpha + a_{0} \nabla \beta + a_{2} \nabla \gamma \right) \cdot \left(\nabla \zeta \right) dx dt \tag{2.9}$$

4. Study of the term on the right-hand-side of (2.7)

Integrating by parts with respect to ξ , using $\psi(-4) = \psi(4) = 0$, and because by construction

$$\phi_{\xi}^{1,\epsilon} = \begin{cases} 0 & \text{if } \xi < -\frac{5}{2} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } -\frac{5}{2} < \xi < -\frac{1}{2} \\ 0 & \text{if } \xi > -\frac{1}{2}, \end{cases}$$

the term on the right-hand-side of (2.7) goes to

$$\lim_{\epsilon \to 0} -\int_{-4}^{4} \int_{0}^{T} \int_{U} \psi \phi^{\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} dx dt d\xi = 3 \int_{0}^{T} \int_{U} \zeta \left(\alpha - \beta \right) dx dt.$$
(2.10)

5. Therefore, letting $\epsilon \to 0$, adding up all the three terms in (2.7), and using an approximation-argument, we conclude that α, β, γ are weak solutions of

$$\frac{3}{2\kappa}\left(-\alpha_t + \beta_t + \gamma_t\right) + \frac{3}{2\kappa}\left(a_{-2}\Delta\alpha - a_0\Delta\beta - a_2\Delta\gamma\right) = 3\alpha - 3\beta,$$

which we may rewrite as

$$(\alpha_t - \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma) = 2\kappa \left(\beta - \alpha\right).$$
(2.11)

6. To get the second equation, repeat the same proof, but this time define

$$\phi^{2,\epsilon}(\xi) := \int_1^{b^2(\xi)} \frac{\tau_\epsilon}{\sigma^\epsilon} d\xi,$$

where

$$b^{2}(\xi) = \begin{cases} -\frac{1}{2} & \text{if } \xi < -\frac{1}{2} \\ \xi & \text{if } -\frac{1}{2} < \xi < \frac{5}{2} \\ \frac{5}{2} & \text{if } \xi > \frac{5}{2}. \end{cases}$$

In that case, using the facts that $\phi^{2,\epsilon}$ goes to $-\frac{3}{2\kappa}$, $-\frac{3}{2\kappa}$, and $\frac{3}{2\kappa}$ uniformly on $\left(-\frac{5}{2},-\frac{3}{2}\right)$, $\left(-\frac{1}{2},\frac{1}{2}\right)$ and $\left(\frac{3}{2},\frac{5}{2}\right)$ respectively, and that

$$\phi_{\xi}^{2,\epsilon} = \begin{cases} 0 & \text{if } \xi < -\frac{1}{2} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } -\frac{1}{2} < \xi < \frac{3}{2} \\ 0 & \text{if } \xi > \frac{3}{2}, \end{cases}$$

we obtain that α, β, γ are weak solutions of

$$\frac{3}{2\kappa}\left(-\alpha_t - \beta_t + \gamma_t\right) + \frac{3}{2\kappa}\left(a_{-2}\Delta\alpha + a_0\Delta\beta - a_2\Delta\gamma\right) = 3\beta - 3\gamma,$$

which becomes

$$(\alpha_t + \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha - a_0\Delta\beta + a_2\Delta\gamma) = 2\kappa(\gamma - \beta).$$
(2.12)

7. Finally, to get the third equation, you can either use the fact that $\gamma = 1 - \alpha - \beta$, or repeat the same proof, but this time defining

$$\phi^{3,\epsilon}(\xi) := \int_{-1}^{b^3(\xi)} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi,$$

where

$$b^{3}(\xi) := \begin{cases} -\frac{5}{2} & \text{if } \xi < -\frac{5}{2}, \\ \xi & \text{if } -\frac{5}{2} < \xi < \frac{5}{2} \\ \frac{5}{2} & \text{if } \xi > \frac{5}{2}, \end{cases}$$

and this time, using that $\phi^{3,\epsilon}$ goes to $-\frac{3}{2\kappa}$, $\frac{3}{2\kappa}$, and $\frac{9}{2\kappa}$ uniformly on $\left(-\frac{5}{2}, -\frac{3}{2}\right)$, $\left(-\frac{1}{2}, \frac{1}{2}\right)$, and $\left(\frac{3}{2}, \frac{5}{2}\right)$ respectively, as well as that

$$\phi_{\xi}^{3,\epsilon} = \begin{cases} 0 & \text{if } \xi < -\frac{5}{2} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } -\frac{5}{2} < \xi < \frac{5}{2} \\ 0 & \text{if } \xi > \frac{5}{2}, \end{cases}$$

we obtain

$$\frac{3}{2\kappa}\left(-\alpha_t+\beta_t+3\gamma_t\right)+\frac{3}{2\kappa}\left(a_{-2}\Delta\alpha-a_0\Delta\beta-3a_2\Delta\gamma\right)=3\alpha-3\gamma,$$

which becomes

$$(\alpha_t - \beta_t - 3\gamma_t) + (-a_{-2}\Delta\alpha + a_0\Delta\beta + 3a_2\Delta\gamma) = 2\kappa(\gamma - \alpha).$$
(2.13)

8. In conclusion, from (2.11) - (2.13), we obtain that α,β,γ are weak solutions of the system

$$\begin{cases} (\alpha_t - \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma) = 2\kappa (\beta - \alpha) \\ (\alpha_t + \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha - a_0\Delta\beta + a_2\Delta\gamma) = 2\kappa (\gamma - \beta) \\ (\alpha_t - \beta_t - 3\gamma_t) + (-a_{-2}\Delta\alpha + a_0\Delta\beta + 3a_2\Delta\gamma) = 2\kappa (\gamma - \alpha) , \end{cases}$$

which, solving for α_t, β_t , and γ_t , gives us the desired reaction-diffusion system

$$\begin{cases} \alpha_t - a_{-2}\Delta\alpha = \kappa \left(\beta - \alpha\right) \\ \beta_t - a_0\Delta\beta = \kappa \left(\alpha - 2\beta + \gamma\right) \\ \gamma_t - a_2\Delta\gamma = \kappa \left(\beta - \gamma\right). \end{cases}$$

9. Finally, we obtain the boundary conditions $\frac{\partial \alpha}{\partial \nu} = \frac{\partial \beta}{\partial \nu} = \frac{\partial \gamma}{\partial \nu} = 0$ on $\partial U \times \mathbb{R} \times [0, T]$ just like we did in chapter 1, and likewise we obtain the initial conditions $\alpha(x, 0) = \alpha_0, \beta(x, 0) = \beta_0, \gamma(x, 0) = \gamma_0$ on U using assumption (2.4).

2.4 Generalization

Introduction

Assume again that H is a triple-well function, but time do not assume that H''(-1) = H''(1) and H''(-2) = H''(0) = H''(2) any more. Notice that H is not necessarily even any more.



Figure 2.4: A generalized triple-well potential function H

In that case, define

$$p := \left(\frac{1}{\sqrt{H''(-2)}} + \frac{1}{\sqrt{H''(0)}} + \frac{1}{\sqrt{H''(2)}}\right)^{-1}, \quad p_i = \frac{p}{\sqrt{H''(i)}}, \quad \kappa^{\pm} := \frac{3p\sqrt{|H''(\pm 1)|}}{2\pi}.$$

Then the proof in the previous section remains unmodified, except that our asymptotic estimate of $e^{-\frac{\bar{H}_e}{\epsilon^2}}$ changes to

$$\begin{split} e^{-\frac{\bar{H}_{\epsilon^2}}{\epsilon^2}} &= \int_{\mathbb{R}} e^{-\frac{H(\xi)}{\epsilon^2}} d\xi \\ &= \int_{-\infty}^{-1} e^{-\frac{H(\xi)}{\epsilon^2}} d\xi + \int_{-1}^{1} e^{-\frac{H(\xi)}{\epsilon^2}} d\xi + \int_{1}^{\infty} e^{-\frac{H(\xi)}{\epsilon^2}} d\xi \\ &= \epsilon \sqrt{2\pi} \left(\frac{1}{\sqrt{H''(-2)}} + \frac{1}{\sqrt{H''(0)}} + \frac{1}{\sqrt{H''(2)}} \right) (1 + o(1)) \\ &= \epsilon \frac{\sqrt{2\pi}}{p} (1 + o(1)), \end{split}$$

and hence

$$e^{\frac{\bar{H}_{\epsilon}}{\epsilon^2}} = \frac{1}{\epsilon} \frac{p}{\sqrt{2\pi}} (1 + o(1)).$$

Study of the density σ^{ϵ}

The only modification to Lemma 7 is that, as $\epsilon \to 0$,

$$\int_{\pm 2-\delta}^{\pm 2+\delta} \sigma^{\epsilon} d\xi \longrightarrow p_{\pm 2} \quad \int_{-\delta}^{\delta} \sigma^{\epsilon} d\xi \longrightarrow p_{0} \quad \int_{\pm 1-\delta}^{\pm 1+\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow \frac{3}{\kappa^{\pm}}.$$

Main theorem

The statement of the main theorem remains unchanged. The only difference in the proof is that, using $\phi^{1,\epsilon}\psi\zeta$ as our test function, we obtain that α, β, γ satisfy

$$\frac{3}{2\kappa^{-}}\left(-\alpha_t+\beta_t+\gamma_t\right)+\frac{3}{2\kappa^{-}}\left(a_{-2}\Delta\alpha-a_0\Delta\beta-a_2\Delta\gamma\right)=\frac{1}{p_{-2}}\alpha-\frac{1}{p_0}\beta,$$

which can be rewritten as

$$\left(\alpha_t - \beta_t - \gamma_t\right) + \left(-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma\right) = \frac{2\kappa^-}{3}\left(\frac{1}{p_0}\beta - \frac{1}{p_{-2}}\alpha\right).$$
(2.14)

Using $\phi^{2,\epsilon}\psi\zeta$, we obtain

$$\frac{3}{2\kappa^+}\left(-\alpha_t - \beta_t + \gamma_t\right) + \frac{3}{2\kappa^+}\left(a_{-2}\Delta\alpha + a_0\Delta\beta - a_2\Delta\gamma\right) = \frac{1}{p_0}\beta - \frac{1}{p_2}\gamma,$$

which becomes

$$(\alpha_t + \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha - a_0\Delta\beta + a_2\Delta\gamma) = \frac{2\kappa^+}{3} \left(\frac{1}{p_2}\gamma - \frac{1}{p_0}\beta\right).$$
(2.15)

Finally, using $\phi^{3,\epsilon}\psi\zeta$, we infer that

$$\frac{3}{2\kappa^{-}}\left(-\alpha_t+\beta_t+\gamma_t\right)+\frac{3}{2\kappa^{+}}\gamma_t+\frac{3}{2\kappa^{-}}\left(a_{-2}\Delta\alpha-a_0\Delta\beta-a_2\Delta\gamma\right)-\frac{3}{2\kappa^{+}}a_2\Delta\gamma=\frac{1}{p_{-2}}\alpha-\frac{1}{p_2}\gamma,$$

which we may rewrite as

$$(\alpha_t - \beta_t - \gamma_t) - 2\left(\frac{\kappa^-}{\kappa^+}\right)\gamma_t + (-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma) + 2\left(\frac{\kappa^-}{\kappa^+}\right)a_2\Delta\gamma$$
$$= \frac{2\kappa^-}{3}\left(\frac{1}{p_2}\gamma - \frac{1}{p_{-2}}\alpha\right). \quad (2.16)$$

Putting (2.14) - (2.16) together, we conclude that

$$\begin{cases} (\alpha_t - \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma) = \frac{2\kappa^-}{3} \left(\frac{\beta}{p_0} - \frac{\alpha}{p_{-2}}\right) \\ (\alpha_t + \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha - a_0\Delta\beta + a_2\Delta\gamma) = \frac{2\kappa^+}{3} \left(\frac{\gamma}{p_2} - \frac{\beta}{p_0}\right) \\ (\alpha_t - \beta_t - \gamma_t) - 2 \left(\frac{\kappa^-}{\kappa^+}\right) \gamma_t + (-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma) + 2 \left(\frac{\kappa^-}{\kappa^+}\right) a_2\Delta\gamma = \frac{2\kappa^-}{3} \left(\frac{\gamma}{p_2} - \frac{\alpha}{p_{-2}}\right) \end{cases}$$

which, after solving for α_t, β_t , and γ_t , ultimately gives us the system of reaction-diffusion equations (the initial and boundary conditions are treated as before)

$$\begin{cases} \alpha_t - a_{-2}\Delta\alpha = \frac{\kappa^-}{3} \left(\frac{\beta}{p_0} - \frac{\alpha}{p_{-2}}\right) \\ \beta_t - a_0\Delta\beta = \frac{\kappa^-}{3} \left(\frac{\alpha}{p_{-2}} - \frac{\beta}{p_0}\right) + \frac{\kappa^+}{3} \left(\frac{\gamma}{p_2} - \frac{\beta}{p_0}\right) & \text{in } U \times [0, T] \\ \gamma_t - a_2\Delta\gamma = \frac{\kappa^+}{3} \left(\frac{\beta}{p_0} - \frac{\gamma}{p_2}\right) \\ \frac{\partial\alpha}{\partial\nu} = \frac{\partial\beta}{\partial\nu} = \frac{\partial\gamma}{\partial\nu} = 0 & \text{on } \partial U \times [0, T] \\ \alpha = \alpha_0, \beta = \beta_0, \gamma = \gamma_0 & \text{on } U \times \{t = 0\}. \end{cases}$$

$$(2.17)$$

Note: Notice that if H''(-2) = H''(0) = H''(2) and H''(-1) = H''(1), then $p_{-2} = p_0 = p_2 := p'$ and $\kappa^- = \kappa^+ := \kappa'$, and (2.17) indeed reduces to (2.6), with $\kappa = \frac{\kappa'}{3p'}$.

Chapter 3

Periodic Wells

3.1 Introduction

Similar to the previous chapter, assume here that $H = H(\xi)$ is a smooth, nonnegative, and even triple-well function defined on $\left[-\frac{5}{2}, \frac{7}{2}\right]$, with H(1) = H(3) = 1, H(2) = H(0) = 0with local maxima at 1 and 3, and local minima at 0 and 2, as well as H increasing on (0, 1), decreasing on (1, 2), increasing on (2, 3), and decreasing on $\left(3, \frac{7}{2}\right)$. Moreover, assume that H''(0) = H''(2) and H''(1) = H''(3). This time, however, identify the points $\xi = -\frac{5}{2}$ and $\xi = \frac{7}{2}$, so H becomes a potential with periodic wells, as in Figure 3.1 on the next page. In order to get a meaningful asymptotic limit, assume furthermore that H is periodic of period 2, so each well of H has the same structure. Of course, to assure that our solutions u^{ϵ} of (1.4) are be periodic with respect to ξ with period 4, we need to guarantee that both a^{ϵ} and our initial conditions u_0^{ϵ} are periodic with respect to ξ with period 4 as well.

In this case, we need to change our notation slightly: Let $\mathbb{T} = \begin{bmatrix} -\frac{5}{2}, \frac{7}{2} \end{bmatrix}$ (with $-\frac{5}{2}$ and $\frac{7}{2}$ identified) and $D = U \times \mathbb{T}$, and define $\sigma^{\epsilon} := e^{\frac{\overline{H_{\epsilon}} - H}{\epsilon^2}}$, where $\overline{H_{\epsilon}}$ is chosen so that

$$\int_{\mathbb{T}} \sigma^{\epsilon} d\xi = \int_{\mathbb{T}} e^{\frac{\overline{H_{\epsilon}} - H}{\epsilon^2}} d\xi = 1,$$

and finally let

$$\kappa := \frac{\sqrt{H''(0) |H''(1)|}}{2\pi}$$

3.2 Estimates

Basic estimates

The basic estimates (1.18) and (1.23) stay the same, and we make the same assumptions (1.37) - (1.38) on the initial conditions.



Figure 3.1: A potential H with periodic wells

Study of the density σ^ϵ

As before, $\int_{\mathbb{T}} \sigma^{\epsilon} d\xi = 1$ and Laplace's method imply

$$e^{-\frac{\bar{H}_{\epsilon}}{\epsilon^2}} = \epsilon \frac{3\sqrt{2\pi}}{\sqrt{H''(0)}} (1 + o(1)),$$

whence

$$e^{\frac{\bar{H_{\epsilon}}}{\epsilon^2}} = \frac{1}{\epsilon} \frac{\sqrt{H''(0)}}{3\sqrt{2\pi}} (1+o(1)).$$

Let $\delta = \epsilon^{\frac{3}{4}}$ be chosen as usual.

Lemma 9. Define $I_{\delta} := (-2 - \delta, -2 + \delta) \cup (-\delta, \delta) \cup (2 - \delta, 2 + \delta)$ and $J_{\delta} := (-1 - \delta, -1 + \delta) \cup (1 - \delta, 1 + \delta)$. As $\epsilon \to 0$, we have that

$$\int_{\pm 2-\delta}^{\pm 2+\delta} \sigma^{\epsilon} d\xi \longrightarrow \frac{1}{3}, \quad \int_{-\delta}^{\delta} \sigma^{\epsilon} d\xi \longrightarrow \frac{1}{3}, \quad \int_{\mathbb{T}\setminus I_{\delta}} \sigma^{\epsilon} d\xi \longrightarrow 0, \quad \sup_{\mathbb{T}\setminus I_{\delta}} \sigma^{\epsilon} \longrightarrow 0$$
(3.1)

$$\inf_{\mathbb{T}\setminus J_{\delta}} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \longrightarrow \infty, \tag{3.2}$$

$$\int_{\pm 1-\delta}^{\pm 1+\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow \frac{3}{\kappa} \qquad \int_{3-\delta}^{3+\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow \frac{3}{\kappa}, \quad \int_{\mathbb{T}\setminus J_{\delta}} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow 0.$$
(3.3)

The proofs are the same, except that we ignore any terms that previously involved H'(2). For example, let us prove (3.2).

Proof of (3.2). If $\xi \in \mathbb{T} \setminus J_{\delta} = \left[-\frac{5}{2}, -1 - \delta\right] \cup \left(-1 + \delta, 1 - \delta\right) \cup \left(1 + \delta, \frac{7}{2}\right]$, then by Taylor expansion, we obtain

$$H(\xi) \le \max(H(1-\delta), H(1+\delta)) \le 1 + o(\delta) - \frac{\delta^2}{2} |H''(1)|,$$

and therefore

$$\begin{split} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} &= \epsilon^2 e^{\frac{1}{\epsilon^2}} e^{\frac{\bar{H}_{\epsilon} - H}{\epsilon^2}} \\ &\geq \left(\frac{1}{\epsilon} \frac{\sqrt{H''(0)}}{3\sqrt{2\pi}} (1 + o(1))\right) \epsilon^2 e^{\frac{1}{\epsilon^2}} e^{\frac{-1 + o(\delta) + \frac{\delta^2}{2}|H''(1)|}{\epsilon^2}} \\ &\geq \left(\frac{\sqrt{H''(0)}}{3\sqrt{2\pi}} (1 + o(1))\right) \epsilon e^{\frac{1}{2}|H''(1)| \left(\frac{\delta}{\epsilon}\right)^2} e^{\frac{o(\delta)}{\epsilon^2}} \\ &\longrightarrow \infty \qquad (by \ (1.27)), \end{split}$$

from which (3.2) and the third part of (3.3) follow.

Compactness lemma

Using Lemma 9, we are now ready to extract a convergent subsequence from ρ^{ϵ} (relabeled as ρ^{ϵ}) such that $\rho^{\epsilon} \stackrel{\star}{\rightharpoonup} \alpha \delta_{-2} + \beta \delta_0 + \gamma \delta_2$ for some functions α, β, γ , with the appropriate estimates. As before, we obtain that, as $\epsilon \to 0$,

Lemma 10.

$$\begin{cases} u^{\epsilon} \to 3\alpha & a.e. \text{ on } U \times \left[-\frac{5}{2}, -1\right) \cup \left(3, \frac{7}{2}\right] \\ u^{\epsilon} \to 3\beta & a.e. \text{ on } U \times \left(-1, 1\right) \\ u^{\epsilon} \to 3\gamma & a.e. \text{ on } U \times \left(1, 3\right) \end{cases}$$

Proof. While the $U \times (-1, 1)$ -case and the $U \times (1, 3)$ -case are the same as before, the $U \times \left[-\frac{5}{2}, -1\right) \cup \left(3, \frac{7}{2}\right]$ -case needs to be modified a bit. In that case, given c such that $-\frac{5}{2} < c < 1$, by repeating the same proof as the other cases but integrating over $\left[-\frac{5}{2}, c\right]$, we can show that, on $U \times \left[-\frac{5}{2}, -1\right)$, $u^{\epsilon} \longrightarrow u$ for some function u = u(x, t). Using $\rho^{\epsilon} = \sigma^{\epsilon} u^{\epsilon}$,

integrating with respect to ξ on $(-2 - \delta, -2 + \delta)$ and using (3.1), we get $u = 3\alpha$. Now given c' with $3 < c' < \frac{7}{2}$, repeating the same proof, but integrating over $(c', \frac{7}{2}]$, we obtain that on $U \times (3, \frac{7}{2}]$, $u^{\epsilon} \longrightarrow v$ a.e. for some (possibly different) function v = v(x, t). Without loss of generality, we can assume that this convergence actually holds for $\xi = -\frac{5}{2}$, that is $u^{\epsilon} \longrightarrow u$ a.e. on $U \times \{\xi = -\frac{5}{2}\}$. Then, because we have identified $\xi = -\frac{5}{2}$ and $\xi = \frac{7}{2}$ we in fact get u = v a.e., and therefore $u^{\epsilon} \longrightarrow 3\alpha$ on $(3, \frac{7}{2}]$ as well.

Note: Without loss of generality, assume that the convergence in Lemma 10 moreover holds a.e. on $U \times \{\xi = -\frac{13}{4}, -\frac{11}{4}, \pm \frac{5}{4}, \pm \frac{3}{4}\}$.

3.3 Main theorem

We are now ready to state and prove our main theorem.

Theorem 4. Using the assumptions (1.37) - (1.38), (1.40) in chapter 1 and assumption (2.5) in chapter 2, but changing (2.4) to

$$\begin{cases} u_0^{\epsilon} \to 3\alpha_0 \ a.e. \ on \ U \times \left\{ \xi = -\frac{13}{4} \right\} \\ u_0^{\epsilon} \to 3\beta_0 \ a.e. \ on \ U \times \left\{ \xi = -\frac{3}{4} \right\} \\ u_0^{\epsilon} \to 3\gamma_0 \ a.e. \ on \ U \times \left\{ \xi = \frac{5}{4} \right\}, \end{cases}$$
(3.4)

and further assuming that $a^{\epsilon} \in C(\mathbb{T})$ and $\xi \mapsto u_0^{\epsilon}(x,\xi,t)$ is \mathbb{T} -periodic, the statement of the main theorem is exactly as in chapter 2, except that this time the corresponding functions α, β, γ are weak solutions of the system of reaction-diffusion equations

$$\begin{cases} \alpha_t - a_{-2}\Delta\alpha = \kappa \left(\beta + \gamma - 2\alpha\right) \\ \beta_t - a_0\Delta\beta = \kappa \left(\alpha + \gamma - 2\beta\right) & in U \times [0, T] \\ \gamma_t - a_2\Delta\gamma = \kappa \left(\alpha + \beta - 2\gamma\right) \\ \frac{\partial\alpha}{\partial\nu} = 0, \frac{\partial\beta}{\partial\nu} = 0, \frac{\partial\gamma}{\partial\nu} = 0 & on \,\partial U \times [0, T] \\ \alpha(x, 0) = \alpha_0, \beta(x, 0) = \beta_0, \gamma(x, 0) = \gamma_0 & in U \end{cases}$$
(3.5)

Proof. The proof is similar to before, except that, on the one hand, we do not need the cutoff function ψ , but, on the other hand, in order to handle boundary-values, we need to make sure that each of our test-functions $\phi^{1,\epsilon}, \phi^{2,\epsilon}, \phi^{3,\epsilon}$ below has the same value at the endpoints $\xi = -\frac{5}{2}$ and $\xi = \frac{7}{2}$.

1. Define

$$\phi^{1,\epsilon}(\xi) := \int_{-1}^{b^1(\xi)} \frac{\tau_\epsilon}{\sigma^\epsilon} d\xi,$$

where

$$b^{1}(\xi) = \begin{cases} -\frac{5}{4} & \text{if } -\frac{7}{2} \leq \xi < -\frac{5}{4} \\ \xi & \text{if } -\frac{5}{4} < \xi < -\frac{3}{4} \\ -\frac{3}{4} & \text{if } -\frac{3}{4} < \xi < \frac{3}{4} \\ -\xi & \text{if } \frac{3}{4} < \xi < \frac{5}{4} \\ -\frac{5}{4} & \text{if } \frac{5}{4} < \xi \leq \frac{5}{2}. \end{cases}$$



Figure 3.2: The functions b^1 , b^2 , and b^3

Given an arbitrary function $\zeta \in C_c^{\infty}(U \times [0, T])$, using $\phi^{1,\epsilon}\zeta$ as our test-function in (1.4), and integrating over $D \times [0, T]$, we get:

$$\int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi - \int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta a^{\epsilon} \left(\Delta u^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi = \int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} \, dx dt d\xi \quad (3.6)$$

2. Study of the first term on the left-hand-side of (3.6)

Using that $\phi^{1,\epsilon}(\xi)$ converges uniformly to $-\frac{3}{2\kappa}$ on $\left(-\frac{5}{2},-\frac{3}{2}\right)$, to $\frac{3}{2\kappa}$ on $\left(-\frac{1}{2},\frac{1}{2}\right)$ and to $-\frac{3}{2\kappa}$ on $\left(\frac{3}{2},\frac{5}{2}\right)$ by (3.3), we conclude that

$$\lim_{\epsilon \to 0} \int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi = \frac{3}{2\kappa} \int_{0}^{T} \int_{U} \left(-\alpha_{t} + \beta_{t} - \gamma_{t} \right) \zeta dx dt \tag{3.7}$$

3. Study of the second term on the left-hand-side of (3.6)

In a similar fashion, we obtain

$$\lim_{\epsilon \to 0} -\int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta \left(\Delta u^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi = \frac{3}{2\kappa} \int_{0}^{T} \int_{U} \left(-a_{-2} \nabla \alpha + a_{0} \nabla \beta - a_{2} \nabla \gamma \right) \cdot \left(\nabla \zeta \right) dx dt.$$
(3.8)

4. Study of the term on the right-hand-side of (3.6)

Integrating by parts with respect to ξ and noticing that there are no boundary terms because $\phi^{1,\epsilon}\left(-\frac{5}{2}\right) = \phi^{1,\epsilon}\left(\frac{7}{2}\right)$ by construction, $\sigma^{\epsilon}\left(-\frac{5}{2}\right) = \sigma^{\epsilon}\left(\frac{7}{2}\right)$ by assumption on H, and $u_{\xi}^{\epsilon}\left(x,t,-\frac{5}{2}\right) = u_{\xi}^{\epsilon}\left(x,t,\frac{7}{2}\right)$ since we have identified $-\frac{5}{2}$ with $\frac{7}{2}$, we get

$$\int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} dx dt d\xi = -\int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi_{\xi}^{1,\epsilon} \zeta \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} dx dt d\xi.$$
(3.9)

Since by construction

$$\phi_{\xi}^{1,\epsilon} = \begin{cases} 0 & \text{if } -\frac{7}{2} \le \xi < -\frac{5}{4} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } -\frac{5}{4} \le \xi < -\frac{3}{4} \\ 0 & \text{if } -\frac{3}{4} \le \xi < \frac{3}{4} \\ -\frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } \frac{3}{4} \le \xi < \frac{5}{4} \\ 0 & \text{if } \frac{5}{4} < \xi \le \frac{7}{2}, \end{cases}$$

the right-hand-side of (3.9) becomes

Putting everything together, we obtain

$$\lim_{\epsilon \to 0} \int_{\mathbb{T}} \int_{0}^{T} \int_{U} \phi^{1,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} dx dt d\xi = \int_{0}^{T} \int_{U} \zeta \left(3\alpha - 6\beta + 3\gamma \right) dx dt.$$
(3.10)

5. Therefore, letting $\epsilon \to 0$ and applying (3.7) - (3.8) and (3.10) to (3.6), as well as an approximation argument, we conclude that α, β, γ are weak solutions of

$$\frac{3}{2\kappa}\left(-\alpha_t + \beta_t - \gamma_t\right) + \frac{3}{2\kappa}\left(a_{-2}\Delta\alpha - a_0\Delta\beta + a_2\Delta\gamma\right) = 3\alpha - 6\beta + 3\gamma,$$

which can be rewritten as

$$(\alpha_t - \beta_t + \gamma_t) + (-a_{-2}\Delta\alpha + a_0\Delta\beta - a_2\Delta\gamma) = 2\kappa (-\alpha + 2\beta - \gamma).$$
(3.11)

6. To get a second identity relating α, β , and γ , repeat the same proof, but this time define

$$\phi^{2,\epsilon}(\xi) := \int_1^{b^2(\xi)} \frac{\tau_\epsilon}{\sigma^\epsilon} d\xi,$$

where

$$b^{2}(\xi) := \begin{cases} \frac{5}{4} & \text{if } -\frac{7}{2} \leq \xi < -\frac{13}{4} \\ -\xi - 2 & \text{if } -\frac{13}{4} < \xi < -\frac{11}{4} \\ \frac{3}{4} & \text{if } -\frac{11}{4} < \xi < -\frac{3}{4} \\ \xi & \text{if } \frac{3}{4} < \xi < \frac{5}{4} \\ \frac{5}{4} & \text{if } \frac{5}{4} < \xi \leq \frac{5}{2}. \end{cases}$$

Using an approximation argument and the facts that

- (1) $\phi^{2,\epsilon}$ goes to $-\frac{3}{2\kappa}$ uniformly on $\left(-\frac{5}{2}, -\frac{3}{2}\right)$, to $-\frac{3}{2\kappa}$ uniformly on $\left(-\frac{1}{2}, \frac{1}{2}\right)$ and to $\frac{3}{2\kappa}$ uniformly on $\left(\frac{3}{2}, \frac{5}{2}\right)$ by (3.3),
- (2) By construction

$$\phi_{\xi}^{2,\epsilon} = \begin{cases} 0 & \text{if } -\frac{7}{2} \leq \xi < -\frac{13}{4} \\ -\frac{\tau_{\epsilon}}{\sigma^{\epsilon}(-\xi-2)} & \text{if } -\frac{13}{4} < \xi < -\frac{11}{4} \\ 0 & \text{if } -\frac{11}{4} < \xi < \frac{3}{4} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } \frac{3}{4} < \xi < \frac{5}{4} \\ 0 & \text{if } \frac{5}{4} < \xi \leq \frac{5}{2} \end{cases}$$

(3) $\sigma^{\epsilon}(-\xi - 2) = \sigma^{\epsilon}(\xi)$ because *H* is even and 2-periodic,

we conclude that α, β, γ are weak solutions of

$$\frac{3}{2\kappa}\left(-\alpha_t - \beta_t + \gamma_t\right) + \frac{3}{2\kappa}\left(a_{-2}\Delta\alpha + a_0\Delta\beta - a_2\Delta\gamma\right) = 3\alpha + 3\beta - 6\gamma,$$

which can be rewritten as

$$(\alpha_t + \beta_t - \gamma_t) + (-a_{-2}\Delta\alpha - a_0\Delta\beta + a_2\Delta\gamma) = 2\kappa (-\alpha - \beta + 2\gamma).$$
(3.12)

7. Finally, to obtain a third relation between α, β , and γ , you can either use the fact that $\gamma = 1 - \alpha - \beta$, or repeat the same proof, but this time defining

$$\phi^{3,\epsilon}(\xi) := \int_{-3}^{b^3(\xi)} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi,$$

where

$$b^{3}(\xi) := \begin{cases} -\frac{13}{4} & \text{if } -\frac{7}{2} \leq \xi < -\frac{13}{4} \\ \xi & \text{if } -\frac{13}{4} < \xi < -\frac{11}{4} \\ -\frac{11}{4} & \text{if } -\frac{11}{4} < \xi < -\frac{5}{4} \\ -\xi - 4 & \text{if } -\frac{5}{4} < \xi < -\frac{3}{4} \\ -\frac{13}{4} & \text{if } -\frac{3}{4} < \xi \leq \frac{5}{2}. \end{cases}$$

Again, by an approximation argument and because

- (1) $\phi^{3,\epsilon}$ goes to $\frac{3}{2\kappa}$ uniformly on $\left(-\frac{5}{2},-\frac{3}{2}\right)$, to $-\frac{3}{2\kappa}$ uniformly on $\left(-\frac{1}{2},\frac{1}{2}\right)$ and to $-\frac{3}{2\kappa}$ uniformly on $\left(\frac{3}{2},\frac{5}{2}\right)$ by (3.3),
- (2) By construction

$$\phi_{\xi}^{3,\epsilon} = \begin{cases} 0 & \text{if } -\frac{7}{2} \leq \xi < -\frac{13}{4} \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} & \text{if } -\frac{13}{4} < \xi < -\frac{11}{4} \\ 0 & \text{if } -\frac{11}{4} < \xi < -\frac{5}{4} \\ -\frac{\tau_{\epsilon}}{\sigma^{\epsilon}(-4-\xi)} & \text{if } -\frac{5}{4} < \xi < -\frac{3}{4} \\ 0 & \text{if } -\frac{3}{4} < \xi \leq \frac{5}{2}, \end{cases}$$

(3) $\sigma^{\epsilon}(-4-\xi) = \sigma^{\epsilon}(\xi)$ because *H* is even and 2-periodic,

we conclude that α, β, γ are weak solutions of the equation

$$\frac{3}{2\kappa}\left(\alpha_t - \beta_t - \gamma_t\right) + \frac{3}{2\kappa}\left(-a_{-2}\Delta\alpha + a_0\Delta\beta + a_2\Delta\gamma\right) = -6\alpha + 3\beta + 3\gamma,$$

which we may rewrite as

$$(-\alpha_t + \beta_t + \gamma_t) + (a_{-2}\Delta\alpha - a_0\Delta\beta - a_2\Delta\gamma) = 2\kappa (2\alpha - \beta - \gamma)$$
(3.13)

8. In conclusion, combining (3.11), (3.12), (3.13), we obtain that α, β, γ satisfy the system of reaction-diffusion equations

$$\begin{cases} (\alpha_t - \beta_t + \gamma_t) + (-a_{-2}\Delta_x\alpha + a_0\Delta_x\beta - a_2\Delta_x\gamma) = 2\kappa (-\alpha + 2\beta - \gamma) \\ (\alpha_t + \beta_t - \gamma_t) + (-a_{-2}\Delta_x\alpha - a_0\Delta_x\beta + a_2\Delta_x\gamma) = 2\kappa (-\alpha - \beta + 2\gamma) \\ (-\alpha_t + \beta_t + \gamma_t) + (a_{-2}\Delta_x\alpha - a_0\Delta_x\beta - a_2\Delta_x\gamma) = 2\kappa (2\alpha - \beta - \gamma). \end{cases}$$

Solving for α_t, β_t , and γ_t , we thereby obtain our desired reaction-diffusion system in $U \times [0, T]$:

$$\begin{cases} \alpha_t - a_{-2}\Delta\alpha = \kappa \left(\beta + \gamma - 2\alpha\right) \\ \beta_t - a_0\Delta\beta = \kappa \left(\alpha + \gamma - 2\beta\right) \\ \gamma_t - a_2\Delta\gamma = \kappa \left(\alpha + \beta - 2\gamma\right). \end{cases}$$

9. The boundary condition $\frac{\partial \alpha}{\partial \nu} = 0, \frac{\partial \beta}{\partial \nu} = 0, \frac{\partial \gamma}{\partial \nu} = 0$ on $\partial U \times [0, T]$ follows as in the previous chapter, and the initial condition $\alpha(x, 0) = \alpha_0(x), \beta(x, 0) = \beta_0(x), \gamma(x, 0) = \gamma_0(x)$ follows from Lemma 10 with t = 0 and assumption (3.4).

Chapter 4

Infinitely-many wells

4.1 Introduction

In this chapter, we assume that $H = H(\xi)$ is a smooth, nonnegative, and even potential function with an infinite number of wells. This means that for every $m \in \mathbb{Z}$, H(2m) = 0, H(2m+1) = 1, with local minima at $\xi = 2m$ and local maxima at $\xi = 2m + 1$, and His increasing on (2m, 2m + 1) and decreasing on (2m - 1, 2m). Finally, assume that H is periodic of period 2, that is, each well of H has the same structure.



Figure 4.1: An infinite-well potential H

Notation: In order to get a nontrivial asymptotic limit, we need to modify our nor-

malization condition on σ^{ϵ} a little bit. Assume that $\sigma^{\epsilon} = e^{\frac{\overline{H_{\epsilon}} - H}{\epsilon^2}}$, where $\overline{H_{\epsilon}}$ is chosen so that

$$\int_{-1}^{1} \sigma^{\epsilon} d\xi = \int_{-1}^{1} e^{\frac{\overline{H_{\epsilon}} - H}{\epsilon^{2}}} d\xi = 1.$$

and let

$$\kappa := \frac{\sqrt{H''(0)\left|H''(1)\right|}}{2\pi}.$$

4.2 Estimates

Basic estimates

The basic estimates (1.18) and (1.23) stay the same, and we make the same assumptions (1.37) and (1.38) on the initial conditions.

Study of the density σ^{ϵ}

In this case, $\int_{-1}^{1} \sigma^{\epsilon} d\xi = 1$ and Laplace's method imply

$$e^{-\frac{\bar{H_{\epsilon}}}{\epsilon^2}} = \int_{-1}^{1} e^{-\frac{H(\xi)}{\epsilon^2}} d\xi = \epsilon \left(\frac{2\sqrt{2\pi}}{\sqrt{H''(0)}}\right) (1+o(1)),$$

and therefore

$$e^{\frac{\bar{H_{\epsilon}}}{\epsilon^2}} = \frac{1}{\epsilon} \left(\frac{\sqrt{H''(0)}}{2\sqrt{2\pi}} \right) (1+o(1)).$$

Define $\delta = \epsilon^{\frac{3}{4}}$ be chosen as usual. The compactness estimates in this case are as follows:

Lemma 11. Let $I_{\delta}^{even} := \bigcup_{m=-\infty}^{\infty} (2m - \delta, 2m + \delta)$ and $I_{\delta}^{odd} := \bigcup_{m=-\infty}^{\infty} (2m + 1 - \delta, 2m + 1 + \delta)$. Then, for every $m \in \mathbb{Z}$, we have, as $\epsilon \to 0$,

$$\sup_{\mathbb{R}\setminus I^{even}_{\delta}} \sigma^{\epsilon} \longrightarrow 0, \quad \int_{\mathbb{R}\setminus I^{even}_{\delta}} \sigma^{\epsilon} d\xi \longrightarrow 0, \quad \int_{2m-\delta}^{2m+\delta} \sigma^{\epsilon} d\xi \longrightarrow 1, \tag{4.1}$$

$$\inf_{\mathbb{R}\setminus I_{\delta}^{odd}} \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} \longrightarrow \infty \tag{4.2}$$

$$\int_{\mathbb{R}\backslash I_{\delta}^{odd}} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow 0, \quad \int_{2m+1-\delta}^{2m+1+\delta} \frac{\tau_{\epsilon}}{\sigma^{\epsilon}} d\xi \longrightarrow \frac{2}{\kappa}.$$
(4.3)

Compactness lemma

Using Lemma 11, we are able to extract a subsequence from ρ^{ϵ} (relabeled as ρ^{ϵ}) with the property that $\rho^{\epsilon} \stackrel{\star}{\rightharpoonup} \sum_{m=-\infty}^{\infty} \alpha^{m} \delta_{2m}$ for some functions $\alpha^{m} \in H^{1}(U \times [0, T]), m \in \mathbb{Z}$, with the corresponding estimates. We also have that for every $m \in \mathbb{Z}$, as $\epsilon \to 0$,

Lemma 12. For all $t \in [0,T]$ and all $m \in \mathbb{Z}$

 $u^{\epsilon}(x,\xi,t) \longrightarrow \alpha^{m}(x,t)$ a.e. on $U \times (2m-1,2m+1)$.

Without loss of generality, assume that the convergence holds a.e. on $U \times \{\xi = 2m \mid m \in \mathbb{Z}\}$.

4.3 Main theorem

Theorem 5. Assume (1.37) - (1.38) as before, but change assumption (1.39) to

$$u_0^{\epsilon} \longrightarrow 2\alpha_0^m \qquad a.e. \ on \ U \times \{\xi = 2m\}$$

$$(4.4)$$

for all $m \in \mathbb{Z}$, where $\alpha_0^m = \alpha_0^m(x)$ are smooth. Furthermore, change assumption (1.41) to

$$a^{\epsilon} \longrightarrow a = a(\xi) \text{ uniformly on } \left(2m - \frac{1}{2}, 2m + \frac{1}{2}\right)$$
 (4.5)

Then, as $\epsilon \to 0$,

$$\rho^{\epsilon}(x,\xi,t) \stackrel{\star}{\rightharpoonup} \sum_{m=-\infty}^{\infty} \alpha^m(x,t) \delta_{2m},$$

where the functions $\alpha^m = \alpha^m(x,t)$ $(m \in \mathbb{Z})$ are weak solutions of the following infinite system of reaction-diffusion equations

$$\begin{cases} \alpha_t^m - a^{2m} \Delta \alpha^m = \kappa \left(\alpha^{m-1} - 2\alpha^m + \alpha^{m+1} \right) & in U \times [0, T], m \in \mathbb{Z} \\ \frac{\partial \alpha^m}{\partial \nu} = 0 & on \, \partial U \times [0, T], m \in \mathbb{Z} \\ \alpha^m(x, 0) = \alpha_0^m & in \, U, m \in \mathbb{Z} \end{cases}$$
(4.6)

CHAPTER 4. INFINITELY-MANY WELLS

Proof. We again do not need the cutoff function ψ , but instead we need to make sure that each test function $\phi^{m,\epsilon}$ below has compact support.

1. Given $m \in \mathbb{Z}$, define

$$\phi^{m,\epsilon}(\xi) := \int_0^{b^m(\xi)} \frac{\tau_\epsilon}{\sigma^\epsilon} d\xi,$$

where

$$b^{m}(\xi) = \begin{cases} 0 & \text{if } \xi < 2m - 2\\ \xi - 2m + 2 & \text{if } 2m - 2 < \xi < 2m - \frac{1}{4}\\ \frac{7}{4} & \text{if } 2m - \frac{1}{4} < \xi < 2m + \frac{1}{4} \\ -\xi + 2m + 2 & \text{if } 2m + \frac{1}{4} < \xi < 2m + 2\\ 0 & \text{if } \xi > 2m + 2. \end{cases}$$



Figure 4.2: The functions b^m

and finally let $\zeta = \zeta(x,t) \in C_c^{\infty}(U \times [0,T])$ be arbitrary.

Using $\phi^{m,\epsilon}\zeta$ as our test-function in (1.4) and integrating on $D \times [0,T]$, we obtain

$$\int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi^{m,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi - \int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi^{m,\epsilon} \zeta a^{\epsilon} \left(\Delta u^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi \\ = \int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi^{m,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} \, dx dt d\xi.$$
(4.7)

2. Study of the first term on the left-hand-side of (4.7)

By (4.3), since $\phi^{m,\epsilon}(\xi)$ converges uniformly to $\frac{1}{\kappa}$ on $(2m - \frac{1}{4}, 2m + \frac{1}{4})$ and to 0 on $(2p - \frac{1}{4}, 2p + \frac{1}{4})$, whenever $p \neq m$, we get

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi^{m,\epsilon} \zeta u_{t}^{\epsilon} \sigma^{\epsilon} \, dx dt d\xi = \frac{1}{\kappa} \int_{0}^{T} \int_{U} \alpha_{t}^{m} \zeta dx dt.$$
(4.8)

3. Study of the second term on the left-hand-side of (4.7)

Likewise, we conclude that

$$\lim_{\epsilon \to 0} -\int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi^{m,\epsilon} \zeta \left(\Delta u^{\epsilon} \right) \sigma^{\epsilon} \, dx dt d\xi = \frac{1}{\kappa} \int_{0}^{T} \int_{U} a^{2m} \left(\nabla \alpha^{m} \right) \cdot \left(\nabla \zeta \right) dx dt. \tag{4.9}$$

4. Study of the third on the right-hand-side of (4.7)

Integrating by parts with respect to ξ and noting that there are no boundary terms because $\phi^{m,\epsilon}(\xi) \equiv 0$ for large ξ , we deduce that

$$\int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi^{m,\epsilon} \zeta \left(\frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \right)_{\xi} \, dx dt d\xi = - \int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi_{\xi}^{m,\epsilon} \zeta \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \, dx dt d\xi$$

Notice that by construction

$$\phi_{\xi}^{m,\epsilon} = \begin{cases} 0 & \text{if } \xi < 2m - 2 \\ \frac{\tau_{\epsilon}}{\sigma^{\epsilon}(\xi - 2m + 2)} & \text{if } 2m - 2 < \xi < 2m - \frac{1}{4} \\ 0 & \text{if } 2m - \frac{1}{4} < \xi < 2m + \frac{1}{4} \\ -\frac{\tau_{\epsilon}}{\sigma^{\epsilon}(-\xi + 2m + 2)} & \text{if } 2m + \frac{1}{4} < \xi < 2m + 2 \\ 0 & \text{if } \xi > 2m + 2, \end{cases}$$

and moreover, since we assumed H to be even and periodic of period 2, we have that $\sigma^{\epsilon}(\xi - 2m + 2) = \sigma^{\epsilon}(\xi)$ and $\sigma^{\epsilon}(-\xi + 2m + 2) = \sigma^{\epsilon}(-\xi) = \sigma^{\epsilon}(\xi)$. Therefore, the right-hand-side of (4.7) becomes

$$\lim_{\epsilon \to 0} -\int_{\mathbb{R}} \int_{0}^{T} \int_{U} \phi_{\xi}^{m,\epsilon} \zeta \, \frac{\sigma^{\epsilon}}{\tau_{\epsilon}} u_{\xi}^{\epsilon} \, dx dt d\xi = \int_{0}^{T} \int_{U} \zeta \left(\alpha^{m-1} - 2\alpha^{m} + \alpha^{m+1} \right) dx dt. \tag{4.10}$$

5. Finally, letting $\epsilon \to 0$ in (4.7) and using (4.8) – (4.10) and an approximation-argument, we conclude that $\alpha^{m-1}, \alpha^m, \alpha^{m+1}$ are weak solutions to the equation

$$\frac{1}{\kappa}\alpha_t^m - \frac{1}{\kappa}a^{2m}\Delta\alpha^m = \alpha^{m-1} - 2\alpha^m + \alpha^{m+1},$$

which can be rewritten as

$$\alpha_t^m - a^{2m} \Delta \alpha^m = \kappa \left(\alpha^{m-1} - 2\alpha^m + \alpha^{m+1} \right).$$

Since $m \in \mathbb{Z}$ was arbitrary, we obtain our desired result.

6. The boundary condition $\frac{\partial \alpha^m}{\partial \nu} = 0$ on $\partial U \times [0, T]$ follows as usual, and the initial condition $\alpha^m(x, 0) = \alpha_0^m(x)$ follows from assumption (4.4) and Lemma 12 with t = 0. Notice in particular that, although we are dealing with an infinite system of reaction-diffusion equations, the usual regularity theory for (finite) linear constant-coefficient systems of parabolic equations still applies because, for fixed $m \in \mathbb{Z}$, the derivative-terms in the m-th equation depend only on α^m .

Bibliography

- L. Ambrosio, N. Gigli, and G. Savaré. Gradient flows in metric spaces and in the space of probability measures. Lectures in Mathematics ETH Zürich. Birkhäuser Verlag, Basel, 2005, pp. viii+333.
- [2] L. Ambrosio, G. Savaré, and L. Zambotti. "Existence and stability for Fokker-Planck equations with log-concave reference measure". In: *Probab. Theory Related Fields* 145.3-4 (2009), pp. 517–564.
- [3] S. Arnrich et al. "Passing to the limit in a Wasserstein gradient flow: from diffusion to reaction". In: *Calc. Var. Partial Differential Equations* 44.3-4 (2012), pp. 419–454.
- [4] S. Arrhenius. Uber die Reaktionsgeschwindigkeit bei der Inversion von Rohrzucker durch Säuren. Wilhelm Engelmann, 1889.
- [5] H. Attouch. Variational convergence for functions and operators. Applicable Mathematics Series. Pitman (Advanced Publishing Program), Boston, MA, 1984, pp. xiv+423.
- [6] J-D Benamou and Y. Brenier. "A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem". In: Numer. Math. 84.3 (2000), pp. 375–393.
- [7] C. Bender and S. Orszag. Advanced Mathematical Methods for Scientists and Engineers. McGraw-Hill, 1978.
- [8] H. Berestycki, J. Bouhours, and G. Chapuisat. "Front blocking and propagation in cylinders with varying cross section". In: ArXiv e-prints (Jan. 2015). arXiv: 1501. 01326 [math.AP].
- [9] H. Berestycki and G. Chapuisat. "Traveling fronts guided by the environment for reaction-diffusion equations". In: Networks and Heterogeneous Media 8.1 (2013), pp. 79– 114.
- [10] H. Berestycki, J Roquejoffre, and L. Rossi. "The Shape of Expansion Induced by a Line with Fast Diffusion in Fisher-KPP Equations". In: *Comm. Math. Phys.* 343.1 (2016), pp. 207–232.
- [11] N. Berglund. "Kramers' law: Validity, derivations and generalisations". In: ArXiv eprints (June 2011). arXiv: 1106.5799 [math.PR].

BIBLIOGRAPHY

- [12] A. Blanchet, V. Calvez, and J. Carrillo. "Convergence of the mass-transport steepest descent scheme for the subcritical Patlak-Keller-Segel model". In: SIAM J. Numer. Anal. 46.2 (2008), pp. 691–721.
- M. Born and J.R. Oppenheimer. "Zur Quantentheorie der Molekeln". In: Ann. Physik 84 (1927), pp. 457–484.
- [14] H. Brézis. Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert. North-Holland Mathematics Studies, No. 5. Notas de Matemática (50). North-Holland Publishing Co., Amsterdam-London; American Elsevier Publishing Co., New York, 1973, pp. vi+183.
- [15] E. Carlen and W. Gangbo. "Solution of a model Boltzmann equation via steepest descent in the 2-Wasserstein metric". In: Arch. Ration. Mech. Anal. 172.1 (2004), pp. 21–64.
- [16] J. Carrillo et al. "Global-in-time weak measure solutions and finite-time aggregation for nonlocal interaction equations". In: *Duke Math. J.* 156.2 (2011), pp. 229–271.
- [17] G. Dal Maso. "An introduction to Γ -convergence". In: Progr. Nonlinear Differential Equations Appl. 8 (1993).
- [18] E. De Giorgi and T. Franzoni. "Su un tipo di convergenza variazionale". In: Atti Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur. 58 (1975), pp. 842–850.
- [19] E. De Giorgi, A. Marino, and M. Tosques. "Problems of evolution in metric spaces and maximal decreasing curve". In: Atti Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur. (8) 68.3 (1980), pp. 180–187.
- [20] E. De Giorgi and S. Spagnolo. "Sulla convergenza degli integrali dell'energia per operatori ellittici del secondo ordine". In: Boll. Un. Mat. Ital. (4) 8 (1973), pp. 391– 411.
- [21] L.C. Evans and P.R. Tabrizian. "Asymptotics for scaled Kramers-Smoluchowski equations". In: SIAM Journal on Mathematical Analysis (to appear) (2016), pp. 1–22.
- [22] P.C. Fife. Mathematical aspects of reacting and diffusing systems. Vol. 28. Lecture Notes in Biomathematics. Springer-Verlag, Berlin-New York, 1979, pp. iv+185.
- [23] R.A. Fisher. "The wave of advance of advantageous genes". In: Annals of Eugenics 7 (1937), pp. 355–369.
- [24] U. Gianazza, G. Savaré, and G. Toscani. "The Wasserstein gradient flow of the Fisher information and the quantum drift-diffusion equation". In: Arch. Ration. Mech. Anal. 194.1 (2009), pp. 133–220.
- [25] N. Gigli. "On the heat flow on metric measure spaces: existence, uniqueness and stability". In: Calc. Var. Partial Differential Equations 39.1-2 (2010), pp. 101–120.
- [26] P. Grindrod. Patterns and waves. Oxford Applied Mathematics and Computing Science Series. The theory and applications of reaction-diffusion equations. The Clarendon Press, Oxford University Press, New York, 1991, pp. x+239.
BIBLIOGRAPHY

- [27] P. Hanggi, P. Talkner, and M. Borkovec. "Reaction-rate theory: Fifty years after Kramers". In: *Rev. Moderm Phys.* 62.2 (1990), pp. 251–342.
- [28] W. Hehre. A guide to molecular mechanics and quantum chemical calculations. Vol. 2. Wavefunction Irvine, CA, 2003.
- [29] M. Herrmann and B. Niethammer. "Kramers' formula for chemical reactions in the context of Wasserstein gradient flows". In: Commun. Math. Sci. 9.2 (2011), pp. 623– 635.
- [30] U. Hornung, ed. Homogenization and porous media. Vol. 6. Interdisciplinary Applied Mathematics. Springer-Verlag, New York, 1997, pp. xvi+275.
- [31] J. Hutchinson. "Second fundamental form for varifolds and the existence of surfaces minimising curvature". In: *Indiana Univ. Math. J.* 35.1 (1986), pp. 45–71.
- [32] R. Jordan, D. Kinderlehrer, and F. Otto. "Free energy and the Fokker-Planck equation". In: *Phys. D* 107.2-4 (1997). Landscape paradigms in physics and biology (Los Alamos, NM, 1996), pp. 265–271.
- [33] B. S. Kerner and V. V. Osipov. Autosolitons. Vol. 61. Fundamental Theories of Physics. A new approach to problems of self-organization and turbulence, With the collaboration of A. Dubitsky [A. L. Dubitskiĭ] (Appendix 1) and E. Kuznetsova (Appendix 2), Translated from the Russian by A. S. Dobroslavsky [A. S. Dobroslavskiĭ]. Kluwer Academic Publishers Group, Dordrecht, 1994, pp. xvi+671.
- [34] H.A. Kramers. "Brownian motion in a field of force and the diffusion model of chemical reactions". In: *Phys.* 7 (1940), pp. 284–304.
- [35] K. Laidler and M. King. "Development of transition-state theory". In: *The Journal of Physical Chemistry* 87.15 (1983), pp. 2657–2664.
- [36] E. Lewars. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics. Introduction to the Theory and Applications of Molecular and. Springer, 2003.
- [37] A.W. Liehr. *Dissipative solitons in reaction diffusion systems*. Springer Series in Synergetics. Mechanisms, dynamics, interaction. Springer, Heidelberg, 2013, pp. xx+212.
- [38] E. S. Lobanova and F. I. Ataullakhanov. "Running Pulses of Complex Shape in a Reaction-Diffusion Model". In: *Phys. Rev. Lett.* 93 (9 2004), p. 098303.
- [39] D. Matthes, R. McCann, and G. Savaré. "A family of nonlinear fourth order equations of gradient flow type". In: Comm. Partial Differential Equations 34.10-12 (2009), pp. 1352–1397.
- [40] A. D. Mcnaught and A. Wilkinson. *IUPAC. Compendium of Chemical Terminology*, 2nd ed. (the "Gold Book"). WileyBlackwell; 2nd Revised edition edition.
- [41] A. Mielke, T. Roubíček, and U. Stefanelli. "Γ-limits and relaxations for rate-independent evolutionary problems". In: *Calc. Var. Partial Differential Equations* 31.3 (2008), pp. 387–416.

BIBLIOGRAPHY

- [42] A. Mielke and U. Stefanelli. "Weighted energy-dissipation functionals for gradient flows". In: ESAIM Control Optim. Calc. Var. 17.1 (2011), pp. 52–85.
- [43] A. S. Mikhaĭlov. *Foundations of synergetics. I.* Second. Vol. 51. Springer Series in Synergetics. Distributed active systems. Springer-Verlag, Berlin, 1994, pp. xii+213.
- [44] J.W. Moore, W.G. Davies, and R.W. Collins. *Chemistry*. McGraw-Hill, 1978.
- [45] B. Niethammer and Y. Oshita. "A rigorous derivation of mean-field models for diblock copolymer melts". In: Calc. Var. Partial Differential Equations 39.3-4 (2010), pp. 273– 305.
- [46] B. Niethammer and F. Otto. "Ostwald ripening: the screening length revisited". In: Calc. Var. Partial Differential Equations 13.1 (2001), pp. 33–68.
- [47] F. Otto. "The geometry of dissipative evolution equations: the porous medium equation". In: Comm. Partial Differential Equations 26.1-2 (2001), pp. 101–174.
- [48] M.A. Peletier, G. Savaré, and M. Veneroni. "Chemical Reactions as Γ-Limit of Diffusion". In: SIAM Review 54.2 (2012), pp. 327–352.
- [49] M. Protter and H. Weinberger. *Maximum principles in differential equations*. Corrected reprint of the 1967 original. Springer-Verlag, New York, 1984.
- [50] H.-G. Purwins, H. U. Bödeker, and A. W. Liehr. "Dissipative solitons in reactiondiffusion systems". In: *Dissipative solitons*. Vol. 661. Lecture Notes in Phys. Springer, Berlin, 2005, pp. 267–308.
- [51] J. Rešetnjak. "The weak convergence of completely additive vector-valued set functions". In: Sibirsk. Mat. Z. 9 (1968), pp. 1386–1394.
- [52] H. Risken. *The Fokker-Planck equation*. Second. Vol. 18. Springer Series in Synergetics. Methods of solution and applications. Springer-Verlag, Berlin, 1989, pp. xiv+472.
- [53] E. Sandier and S. Serfaty. "Gamma-convergence of gradient flows with applications to Ginzburg-Landau". In: Comm. Pure Appl. Math. 57.12 (2004), pp. 1627–1672.
- [54] G. Savaré. "Gradient flows and diffusion semigroups in metric spaces under lower curvature bounds". In: C. R. Math. Acad. Sci. Paris 345.3 (2007), pp. 151–154.
- [55] S. Serfaty. "Gamma-convergence of gradient flows on Hilbert and metric spaces and applications". In: *Discrete Contin. Dyn. Syst.* 31.4 (2011), pp. 1427–1451.
- [56] J. Smoller. Shock waves and reaction-diffusion equations. Second. Vol. 258. Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]. Springer-Verlag, New York, 1994, pp. xxiv+632.
- [57] S. Spagnolo. "Sul limite delle soluzioni di problemi di Cauchy relativi all'equazione del calore". In: Ann. Scuola Norm. Sup. Pisa (3) 21 (1967), pp. 657–699.
- [58] S. Spagnolo. "Sulla convergenza di soluzioni di equazioni paraboliche ed ellittiche." In: Ann. Scuola Norm. Sup. Pisa (3) 22 (1968), 571-597; errata, ibid. (3) 22 (1968), p. 673.

- [59] U. Stefanelli. "The Brezis-Ekeland principle for doubly nonlinear equations". In: *SIAM J. Control Optim.* 47.3 (2008), pp. 1615–1642.
- [60] C. Villani. *Topics in optimal transportation*. Vol. 58. Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, 2003, pp. xvi+370.
- [61] Wikipedia. A simple reaction coordinate diagram. [Online; accessed 04-15-2015]. 2008. URL: https://commons.wikimedia.org/wiki/File:Rxn_coordinate_diagram_5. PNG.
- [62] Wikipedia. Potential Energy Surface and Corresponding 2-D Reaction Coordinate Diagram derived from the plane passing through the minimum energy pathway between A and C and passing through B. [Online; accessed 10-27-2013]. 2013. URL: https:// commons.wikimedia.org/wiki/File:Potential_Energy_Surface_and_Corresponding_ Reaction_Coordinate_Diagram.png#metadata.
- [63] Y.B. Zeldovich and D.A. Frank-Kamenetsky. "Towards the theory of uniformly propagating flames". In: Acta Physicochim. CONT 9 (1938), p. 341.