INTEGRO-DIFFERENTIAL EQUATIONS IN MATERIALS SCIENCE

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Abstract

This thesis deals with nonlocal models for solid-solid phase transitions, such as ferromagnetic phase transition or phase separation in binary alloys. We discuss here, among others, nonlocal versions of the Allen-Cahn and Cahn-Hilliard equations, as well as a nonlocal version of the viscous Cahn-Hilliard equation. The analysis of these models can be motivated by the fact that their local analogues fail to be applicable when the wavelength of microstructure is very small, e.g. at the nanometre scale. Though the solutions of these nonlocal equations and those of the local versions share some common properties, we find many differences between them, which are mainly due to the lack of compactness of the semigroups generated by nonlocal equations.

Directly from microscopic considerations, we derive and analyse two new types of equations. One of the equations approximately represents the dynamic Ising model with vacancy-driven dynamics, and the other one is the vacancy-driven model obtained using the Vineyard formalism. These new equations are being put forward as possible improvements of the local and nonlocal Cahn-Hilliard models, as well as of the mean-field model for the Ising model with Kawasaki dynamics.

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Chapter 1

Introduction

1.1 Introduction

Almost all the metallic materials used in engineering applications are alloys, which are mixtures of two or more metallic elements. Alloys may vary in complexity from binary mixtures, e.g. mixtures of copper and zinc or aluminium and iron, to the very complex ones, such as the modern steels. Unlike pure materials, alloys present some interesting properties related to pattern formation and growth of domains within the solid material. These domains may be defined as regions where certain properties of the material deviate from the properties of the bulk of the material. In spite of the wide variety of solid solutions, it is possible to identify some common features, such as the tendency to precipitate or to order at low temperatures. These phenomena take place because there are unequal interactions between different kinds of atoms in their composition. However, metallic alloys are characterized by a tendency to a final state, called the equilibrium state, which should meet the condition of the minimal Helmholtz free energy. Clearly, the length scales on which such phenomena occur depend on the properties of each material, but the mechanisms are universal and allow a general approach to understanding the microstructure.

A wide variety of phase transformations in solids occur below a critical temperature T_c at which, in the absence of an external field, two or more thermody-

namic states are stabilized in physically distinguishable domains and separated from another by mobile domain boundaries. Materials that illustrate this principle include ferromagnets, binary alloys, ferroelectrics, ferroelastics, liquid crystals and superconductors.

The purpose of this thesis is to examine some models of solid-solid phase transitions. We discuss here the nonlocal versions of the well known Allen-Cahn, Cahn-Hilliard and viscous Cahn-Hilliard equations, as well as the mean-field equations derived from Statistical Mechanics, for the Ising model with vacancy-mediated diffusion.

The Allen-Cahn and Cahn-Hilliard equations have been employed to study the kinetics of atomic ordering and compositional phase separation in binary mixtures. They have been very successful in predicting the sequence of phase transformations as well as the kinetics of domain coarsening. These equations can be derived by considering gradient flows of the free energy of the system (the Ginzburg-Landau functional) with respect to an appropriately chosen inner product.

Recently, it was suggested in [66] that the Cahn-Hilliard equation does not reproduce faithfully the details of phase separation when the forces driving the process operate at very short length scales. One can try to avoid this problem by considering instead gradient flows of a different free energy functional, namely the Khachaturyan [68] (or the van der Waals [97]) free energy functional. The new equations can be regarded as the nonlocal versions of the above mentioned equations and have been studied in, among others, [5], [6], [8], [9], [32], [42], [43]. Both approaches describe the rate of change of the order parameter being linearly proportional to the thermodynamic driving force.

In [86], O. Penrose suggested that the function contained within this functional cannot be regarded as the thermodynamic free energy density since this function is not convex, and this contradicts the general theory of *Statistical Mechanics*. Moreover, this approach does not allow one to determine the rate parameter that appears in these equations (the mobility). Using a mean-field type of approximation, he derived the average behaviour of the Ising model with two kinds of dynamics: the Glauber (spin-flip) stochastic dynamics and the Kawasaki (direct

exchange) dynamics. These two new models were compared in [86] with the discrete versions of the Allen-Cahn and Cahn-Hilliard models, and were put forward as possible improvements of the latter ones.

A more realistic representation of the diffusion process in real alloys has been considered in [98], [99] (for the non-conserving order parameter case) and in [49], [50], [101] (for the conserving order parameter case), where a very small number of vacancies is introduced in the system and the atoms are allowed to change places only if a neighbouring lattice site is empty. Monte Carlo simulations were performed for both the usual Ising models and vacancy-driven dynamics, showing that the domain growth regime is reached faster with the vacancy mechanism.

We organize this thesis as follows. In the remainder of this chapter we discuss the phase separation phenomenon and present the Ising model, the mean-field models derived by O. Penrose in [86], and Vineyard's formalism contained in [96].

Chapter 2 contains some background material on the theory of dynamical systems theory and the descriptions of the Allen-Cahn, Cahn-Hilliard and Novick-Cohen-Pego models.

The original material of this thesis is contained in Chapters 3 to 5. In Chapter 3, we discuss the nonlocal Allen-Cahn equation. This chapter has two main parts. The first one focusses on proving that unlike the Allen-Cahn equation, this equation has the property that its solutions do not coarsen when any of the two parameters, one representing the strength of intermolecular forces and the other one the interaction length, is small enough. This result is a consequence of the maximum principle that this equation obeys. The second main part is to approximate the flow generated by the nonlocal Allen-Cahn equation by truncating the free energy functional and then taking the Padé approximants. In this way we derive new equations, which are well posed for both positive and negative time, and solutions to these equations will approximate the solution to the nonlocal Allen-Cahn equation. In the end of the chapter numerical results are shown and discussed.

Chapter 4 deals with three nonlocal mass-conserving models. The equations in discussion are: the mass-conserving version of the nonlocal Allen-Cahn equation,

the nonlocal version of the Cahn-Hilliard equation and the nonlocal extension of the viscous Cahn-Hilliard equation. We show that each of these equations generates semi-dynamical systems in appropriate function spaces. The stationary solutions of these models satisfy the same equation, and some of their properties are discussed here. As in the case of the nonlocal Allen-Cahn equation, it appears that the solutions to these equations do not coarsen if the strength or the length of interactions is small enough. Numerical evidence for this fact is given at the end of this chapter. However, the comparison principle tool used to prove the similar property for the Allen-Cahn equation is no longer available in this case.

In the beginning of Chapter 5 we introduce the system of equations which approximately represents the Ising model with vacancy driven dynamics, then we introduce the mean-field equation derived by using the Vineyard approach. We perform some numerics and compare them with the numerical results for the Penrose equation which approximately represents the Ising model with Kawasaki dynamics.

The thesis concludes with a discussion of the main results and some suggestions for further work.

1.2 Phase transitions in solids

In many physical *systems*, e.g. a piece of iron that under certain conditions can be magnetized, or an alloy that can exist as a mixture of two or more components, one encounters analytic discontinuities or singularities in one of the thermodynamic functions, such as the free energy of the system, which correspond to the occurrence of various kinds of phase transitions.

Phase transitions occur when a material undergoes a spontaneous conversion from one phase to another, at a characteristic temperature. We can speak about solid-solid phase transitions when a rearrangement of molecules that results in a change in the material's lattice structure takes place. The most common examples of phase transitions in solids are: the transition from a normal conductor to a super-conductor, various phenomena associated with the coexistence of phases in

the neighbourhood of a critical point, the behaviour of mixtures and solutions (such as the phase separation phenomena), phenomena of ferromagnetism and antiferromagnetism, the order-disorder transitions in alloys (the tendency of an ordered arrangement to disorder) etc.

Under certain favourable circumstances, one can observe that below a particular temperature T_c a large number of microscopic constituents of a given system may exhibit a tendency to interact with one another in a strong fashion, giving rise to some portions of the system that coexist at different conditions, called *phases*, each portion having homogeneous composition and properties, and being distinct from other parts of the system. The temperature T_c is known as the *critical temperature* of the system and the phases are assumed to be characterized by different values of a dimensionless physical quantity called an *order parameter.* The phase transition process may or may not be affected by some conservation laws, and thus we may speak of a nonconserved order parameter (NCOP) if no global constraints are imposed on the order parameter, and of a conserved order parameter (COP), if such constraints (e.g., mass conservation) are imposed. An example of NCOP phase transition is the phenomenon of *ferromagnetism*, which can be defined as the development of extremely strong magnetic properties in certain materials which occurs when magnetic domains (regions at most 1 mm in dimension) become aligned in the absence of an applied field, below a temperature known as the Curie temperature. It is believed to be caused by magnetic fields generated by the electrons' spins in combination with a mechanism known as exchange coupling, which aligns all the spins in each magnetic domain. The order parameter for this phenomenon is the *magnetization.* As an example of COP phase transition we mention the phase separation of a binary alloy below a critical value of the temperature. In this case the order parameter can be considered to be the concentration of one of the two components. This phenomenon will be described in detail in the next section.

The *homogeneous state* defines that state of the system for which all the parts of the system are alike, while in the *inhomogeneous state* we can find some parts which are different from the others. We call *components* of a certain system the distinct elements or chemical compounds which make up the system.

The study of phase transitions is concerned with how one or more phases in the system change into a new phase or mixture of phases. The dynamics of a particular system may always be viewed under two perspectives: a macroscopic one, where the behaviour of the system is viewed as a whole, and a microscopic one, where each individual atom or molecule is represented.

If the thermodynamic function that exhibits discontinuities or singularities is the free energy of the system, then we can talk about different types of phase transitions, depending on the order of discontinuity in the derivatives of the free energy. When there is a finite discontinuity in one or more of the first derivatives of the free energy with respect to temperature, the transition is called *first order transition.* If the first derivatives are continuous but the second, or third, ... derivative is discontinuous or infinite, the transitions will be regarded as *higher order*, *continuous*, or *critical.* The first classification has been made by Ehrenfest [33], who called the phase transitions after their order of discontinuity, i.e. *first-*, *second-*, *third-*, ... *order transitions.* For further details one can also consult [30], [31], [61], [83], [87], [102].

1.2.1 Phase separation

When a molten alloy is suddenly cooled ("quick quenching"), the homogeneous state is no longer stable and the components of the system, previously perfectly mixed, show a tendency to separate into spatially separated multi-phase structures; in this case we say that phase separation takes place. Let us consider the case of a molten binary alloy, with species α and β of concentrations c_α and c_β, respectively. Since the concentration is a conserved quantity, we have

$$c_\alpha + c_\beta = \text{constant} \tag{1.2.1}$$

at each point of the domain. A useful tool for discussing the phase separation phenomenon is the *phase diagram* represented in Figure 1.1. This diagram allows us to map out what happens with the system under different values of concentration c and temperature T.

Suppose that initially the mixture is at a high temperature, at the point P of

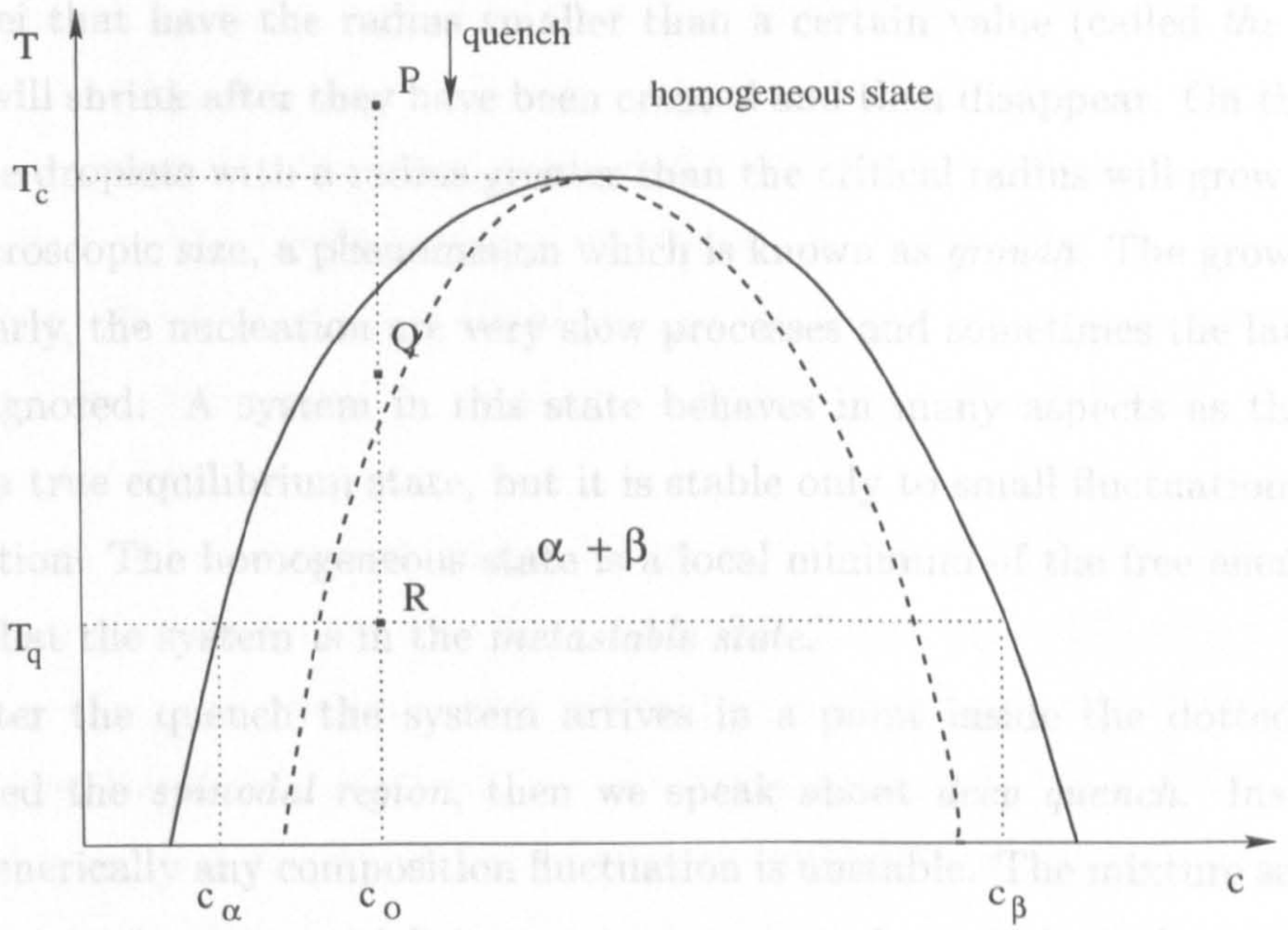

Figure 1.1: Idealized phase diagram for phase separation in binary alloys.

the diagram, having a given concentration c_0. At this point and for all the points lying outside the continuous curve the equilibrium state is the homogeneous state which is stable to all perturbations which do not change the average concentration, and thus there is no phase transition. When the temperature is lowered to some value below the critical point T_c, where the system finds itself in a point inside the region enclosed by the continuous curve, the equilibrium state can no longer be the homogeneous state, but consists of two phases, which coexist and have different values for the concentration. This region is called the *coexistence region* and the full line curve is the *coexistence curve*.

The part of the coexistence region the system arrives in after the quench has a profound effect on the dynamics of the phase separation process. If the mixture arrives at a point that is in the region enclosed by the dotted curve and the continuous one (the *metastable region*), such as the point Q, then we say that the system has suffered a *shallow quench*. In this case the separation process is likely to proceed firstly by the formation of small roughly spherical droplets of one of the two phases, a phenomenon that is known as *nucleation*. It turns out that all

the nuclei that have the radius smaller than a certain value (called *the critical radius*) will shrink after they have been created and then disappear. On the other hand, the droplets with a radius greater than the critical radius will grow in time to a macroscopic size, a phenomenon which is known as *growth*. The growth and, particularly, the nucleation are very slow processes and sometimes the latter one can be ignored. A system in this state behaves in many aspects as though it were in a true equilibrium state, but it is stable only to small fluctuations in the composition. The homogeneous state is a local minimum of the free energy, and we say that the system is in the *metastable state*.

If after the quench the system arrives in a point inside the dotted curve, also called the *spinodal region*, then we speak about *deep quench*. Inside this region generically any composition fluctuation is unstable. The mixture separates out into two phases, one rich in α components and one rich in β components, a phenomenon known as *spinodal decomposition*. For a generic point R inside the spinodal region we find different values for the concentration, c_α and c_β. As time passes, the typical domain size grows in time as the larger domains grow at the expense of small domains, which shrink and disappear. This process of disappearance of the fine structure in time is called *coarsening* (or *Ostwald ripening*). Additional details concerning phase separation can be found, among other places, in [55], [86].

1.2.2 The Ising model

The Ising model is one of the pillars of statistical mechanics and it is the prototype model for all magnetic phase transitions. It was first studied by Lenz [72] and Ising [67] in 1925, as a model of a ferromagnet or antiferromagnet on a crystal lattice. The Ising model tries to imitate behaviour in which a collection of individual elements (e.g., atoms, animals, social behaviour, etc.) modify their behaviour in time so as to conform to the behaviour of other individuals in their vicinity. It has been also used successfully to describe the decomposition of a binary alloy, originally in homogeneous state, into domains of two phases. In biology, it can model neural networks, flocking birds, or beating heart cells.

We consider a lattice Λ populated by two sorts of spins, 'up' and 'down', (or two sorts of atoms, say A and B, for a binary alloy). At each lattice site k we assign an occupation variable σ_k which can take only two values, $\sigma_k = +1$ if the spin at site k is 'up' (respectively, if we find an A-atom at site k), and $\sigma_k = -1$ if the spin is 'down' (for a B-atom at site k). Each spin (atom) can interact with an external magnetic field, H_k, that varies from site to site and with other spins (atoms) in the lattice.

There are various kinds of dynamics that can be considered here. The simplest one is the so-called *Glauber dynamics*, where the spins can just flip from one sign to another. This mechanism cannot be used to model phase separation in binary alloys, where the order parameter is a conserved quantity in the system. Another type of dynamics is the direct interchange between two neighbouring spins, also called *Kawasaki dynamics*, which can also be used as a mechanism for atom migration. When a small number of vacancies are present in the lattice, we can imagine vacancy-mediated dynamics, where an atom can exchange places only with a neighbouring empty site.

If only nearest neighbour interactions are considered in the lattice, and we denote by J_{kl}, K_{klm}, ... the exchange interactions between, respectively, two, three, ... nearest neighbour spins (atoms), then we can write the general Hamiltonian as follows:

$$H = -\sum_{k\in\Lambda} H_k\sigma_k - \frac{1}{2}\sum_{<k,l>} J_{kl}\sigma_k\sigma_l - \frac{1}{6}\sum_{<k,l,m>} K_{klm}\sigma_k\sigma_l\sigma_m - \dots \qquad (1.2.2)$$

where $< \cdot >$ means that the sums are considered over the nearest neighbour pairs, triplets, ... In the absence of an external magnetic field and if we restrict ourselves to pair exchange interactions only, (1.2.2) becomes

$$H = -\frac{1}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)} J_{kl}\sigma_k\sigma_l, \qquad (1.2.3)$$

where $N(k)$ denotes the set of nearest neighbours to site k.

If J is positive, then H decreases for parallel spins (if $A-A$ and $B-B$ bonds are created), fact which corresponds to ferromagnetism (the phase separation into A-rich and B-rich regions), but if J is negative the system will tend to order

(antiferromagnetism), to maximize the number of $A-B$ bonds. For more details one can consult [61], [72], [83], [102].

1.2.3 The Penrose models

Unlike macroscopic models, microscopic models do include representations of each atom in the system, and it is assumed that the kinetics of atomic ordering in binary alloys can be specified by finding the rate at which each atom of the given components will move from one lattice site to another. Since very few models in Statistical Mechanics can be solved exactly, in most cases one has to use approximate methods. One of the most used methods is the *mean-field approximation*, in which the basic assumption is the statistical independence of the local ordering, i.e., of nearest neighbour spins or atoms. In this theory, the order parameter is replaced by its expected value ('mean field' term) and fluctuations about that value are ignored. One has to find the evolution equation for this value.

In order to avoid the derivation of models for phase separations in solids as gradient flows of a free energy functional, which sometimes does not satisfy the convexity requirement of Statistical Mechanics theory, Penrose [85] has derived new types of equations using only Statistical Mechanics principles. He derived two equations which approximately represent the dynamic Ising model with atomic exchange in the mean-field approximation. Two kinds of stochastic dynamics were considered: the spin-flip dynamics of Glauber for the non-conserving order parameter case, and the spin-exchange dynamics of Kawasaki for the conserving case. In these models one solves deterministic equations for the expectation of site occupation as a function of time. It was shown that these equations also have a Lyapunov function, which is not quite the free energy of the system in the mean-field approximation, but this approach has the advantage that it contains no adjustable parameters or functions.

Let us consider an Ising model on a lattice Λ with occupation numbers $\sigma_i = \pm 1$ and assume only interactions between the nearest neighbour spins. Then the energy of the system will be given by (1.2.3). In the case of *Glauber dynamics*

each spin $k \in \Lambda$ has a probability $\omega_k(\sigma)$ per unit time of reversing its sign, and the evolution of the occupation of site k can be expressed as

$$\frac{d}{dt}\mathbf{E}(\sigma_k) = -2\mathbf{E}[\sigma_k \omega_k(\sigma)], \tag{1.2.4}$$

where $\mathbf{E}$ represents the expected value of the spin.

In the case of *Kawasaki dynamics*, for each pair of nearest neighbour sites $< k, l >$, there is a probability $\omega_{kl}(\sigma)$ per unit time that the atom situated at site l swaps with the atom at site k. The corresponding law is

$$\frac{d}{dt}\mathbf{E}(\sigma_k) = \sum_{l \in N(k)} \mathbf{E}[(\sigma_l - \sigma_k)\omega_{kl}(\sigma)], \tag{1.2.5}$$

where $N(k)$ denotes the set of nearest neighbours to site k.

Penrose substituted *Glauber's hyperbolic tangent rule* (see also [54], [92]) into the time evolution equations, which resulted in a differential equation involving the expectation of some nonlinear functions (e.g., the hyperbolic tangent) and some expectations of type $\mathbf{E}(\sigma_k \sigma_l)$. If we suppose that all such spins take values independently of the other spin values, then we can approximate these terms by $\mathbf{E}(\sigma_k)\mathbf{E}(\sigma_l)$, and the average of the nonlinear function by the function at the average value of the argument. The Glauber rule is

$$\omega(\sigma) = \frac{1}{2}\{1 - \tanh[\frac{1}{2}\beta\delta W(\sigma)]\}, \tag{1.2.6}$$

where $\delta W(\sigma)$ is the change in the energy brought about by the transition and $\beta = \frac{1}{\kappa T}$ (κ is the Botzmann's constant and T is the inverse temperature). This rule is a convenient choice of the transition rates $\omega_k(\sigma)$ and $\omega_{kl}(\sigma)$ to satisfy the *detailed balance conditions*

$$\omega_k(\sigma)e^{-\beta W(\sigma)} = \omega_k(\sigma^k)e^{-\beta W(\sigma^k)} \tag{1.2.7}$$

and, respectively,

$$\omega_{kl}(\sigma)e^{-\beta W(\sigma)} = \omega_{kl}(\sigma^{kl})e^{-\beta W(\sigma^{kl})}, \tag{1.2.8}$$

where σ^k is the configuration $(\sigma_1, \sigma_2, \ldots, -\sigma_k, \ldots, \sigma_n)$ when the configuration σ is $(\sigma_1, \sigma_2, \ldots, \sigma_k, \ldots, \sigma_n)$, and the configuration σ^{kl} is obtained from σ by interchanging the spins σ_k and σ_l.

After all these substitutions into the time evolution equations (1.2.4) and (1.2.5), we get

$$\frac{du_k}{dt} = -u_k + \tanh v_k \tag{1.2.9}$$

for Glauber dynamics, and

$$\frac{du_k}{dt} = \frac{1}{2}\sum_{l\in N(k)} \{u_l - u_k + (1 - u_k u_l)\tanh \beta[v_k - v_l + J_{kl}(u_k - u_l)]\} \tag{1.2.10}$$

for Kawasaki dynamics. Here we have set

$$u_k = \mathbf{E}(\sigma_k) \quad \text{and } v_k = \sum_{l\in N(k)} J_{kl}u_l, \quad \text{for all } k \in \Lambda.$$

Note that in the case of Kawasaki dynamics the total number of the atoms of each species is conserved, that is we have

$$\sum_{k\in\Lambda} u_k = const. \tag{1.2.11}$$

The kinetic equation (1.2.9) was also obtain by Suzuki and Kubo in [92]. Each of these approximate kinetic equations have a Lyapunov function; for (1.2.9) this is

$$L_G(u) = \frac{1}{\beta}\sum_{k\in\Lambda}\phi(u_k) - \frac{1}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)} J_{kl}u_k u_l, \tag{1.2.12}$$

where

$$\phi(u) = \frac{1}{2}(1+u)\ln(1+u) + \frac{1}{2}(1-u)\ln(1-u). \tag{1.2.13}$$

For (1.2.10) a Lyapunov function exists provided J_{kl} have the same value for all k, $l \in \Lambda$, say J. Then the Lyapunov function is

$$L_{Kaw}(u) = \frac{1}{\beta}\sum_{k\in\Lambda}\phi(u_k) - \frac{J}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)} u_k u_l - \frac{J}{2}\sum_{k\in\Lambda} u_k^2. \tag{1.2.14}$$

Penrose [85] has also suggested a way of deriving (1.2.9) and (1.2.10) from, respectively, the discrete versions of the Allen-Cahn and the Cahn-Hilliard equations. Concerning (1.2.9), it was shown [37] that there is a critical temperature, T_c, so that for temperatures higher than T_c the uniform state is the unique equilibrium, while below this value there are multiple equilibria. Also, properties of the global dynamics, the bifurcation problem and numerical computations are

discussed in this paper. Simulations for (1.2.10) were performed in [66], showing that this model does reproduce the variations of the wavelength and amplitude with time observed experimentally during the phase separation, even though it fails to describe the very early stages of the decomposition. In Chapter 5 we will be using these techniques to get the approximate equations for the Ising model in which the diffusion process is mediated by a small number of vacancies introduced in the system.

1.2.4 The Vineyard approach

In 1956, G. Vineyard [96] proposed a more general approach for the kinetics of order-disorder transformations, which can be used for alloys having any number of components and, like the Penrose models, this model avoids the use of a bulk free energy functional. The ordering process is described by a set of multiparticle time-dependent distribution functions. Away from equilibrium, all these distribution functions will change with time as atomic exchanges take place on the lattice. The kinetic equations can be written with respect to any n-particle set of distribution functions (where n is the number of particles in a given cluster), depending on the level of approximation. The changing rates of these distribution functions are proportional to the exponential of activation energy for the atomic diffusion jumps. This model can be used for many different mechanisms of atom migration, such as direct exchange or vacancy mechanism. We shall describe briefly here the model for direct exchange mechanism (Kawasaki dynamics) in a binary alloy.

Let Λ be a lattice, in which to each site x corresponds a set of nearest neighbour sites $N(x)$, and the sites are denoted by $x + \delta$. The lattice is populated by two sorts of atoms only, say A and B, with corresponding probabilities $P_A(x;\, t)$ and $P_B(x;\, t)$ at a given time t. Then we have

$$P_A(x;\, t) + P_B(x;\, t) = 1, \quad \text{for all lattice sites } x \text{ and at all times } t. \tag{1.2.15}$$

Let us denote by $P_{AB\{X\}}(x, x + \delta, \{y\};\, t)$ the probability of finding simultaneously an A-atom at x, a B-atom at site $x + \delta$ and the set of atoms $\{X\}$ on the neighbouring sites $\{y\}$, at a particular time t. Also, we denote by $R_{AB}(\{X\})$ the

rate at which these two atoms will exchange places, under the influence of the nearest neighbours around the pair. Similarly, we define $P_{BA\{X\}}(x, x+\delta, \{y\}; t)$ and $R_{BA}(\{X\})$. Then the law for the rate of change of $P_A(x; t)$ is:

$$\frac{d}{dt}P_A(x; t) = \sum_{\delta}\sum_{\{X\}} P_{BA\{X\}}(x, x+\delta, \{y\}; t)R_{BA}(\{X\}) - \\ - \sum_{\delta}\sum_{\{X\}} P_{AB\{X\}}(x, x+\delta, \{y\}; t)R_{AB}(\{X\}). \quad (1.2.16)$$

The equation for $\frac{d}{dt}P_B(x; t)$ is now easily obtained from (1.2.15). These equations cannot be solved analytically unless we simplify somehow the right hand side expressions. One can do this if we assume statistical independence among occupation probabilities. For example, we approximate

$$P_{AB\{X\}}(x, x+\delta, \{y\}; t) \cong P_A(x; t)P_B(x+\delta; t)P_{X_1}(y_1)\ldots P_{X_n}(y_n),$$

where each y_i is an individual site in the set $\{y\}$, and X_i is an atom (A or B) or a vacancy occupying y_i ($i = 1\ldots n$). With this single site approximations, it remains only to specify the jump rates $R_{AB}(\{X\})$, which contain all the physics of the problem. Following Vineyard, we consider an $A-B$ pair situated at $(x,\ x+\delta)$, and we suppose that around the site x we find $n_A(x)$ nearest neighbour atoms of type A, $n_B(x)$ other nearest neighbour atoms of type B, and similar numbers, $n_A(x+\delta)$ and $n_B(x+\delta)$, around the site $x+\delta$. Obviously, for any site x we have

$$n_A(x) + n_B(x) = n_A(x+\delta) + n_B(x+\delta) := z - 1, \quad (1.2.17)$$

where z is the number of all nearest neighbour sites of a given site (the coordination number). We denote by J_{AA}, J_{AB}, J_{BA} and J_{BB} the bond energies between the nearest neighbour atoms $A-A$, $A-B$, $B-A$ and $B-B$, respectively, where all these energies are considered to be non-negative. We assume that $J_{AB} = J_{BA}$ and introduce the quantity $\varepsilon = (J_{AA} + J_{BB} - 2J_{AB})/2$. Clearly, $\varepsilon > 0$ for an ordering system. The energy of a configuration is the sum of all bond energies in the system. The contribution of the pair $A-B$ situated at $(x,\ x+\delta)$ to the total energy is

$$n_A(x)J_{AA} + (z-1-n_A(x))J_{AB} + n_A(x+\delta)J_{BA} + (z-1-n_A(x+\delta))J_{BB},$$

and after the exchange the contribution will be

$$n_A(x)J_{AB} + (z-1-n_A(x))J_{BB} + n_A(x+\delta)J_{AA} + (z-1-n_A(x+\delta))J_{BA}.$$

Thus the net change in the energy due to this pair is

$$\Delta E(x,\, x+\delta) = 2\varepsilon(n_A(x+\delta - n_A(x)),$$

and Vineyard concluded that the exchange rate $R_{AB}(\{X\})$ is of the form

$$R_{AV}(\{X\}) = \nu e^{-\beta(U+\varepsilon(n_A(x+\delta)-n_A(x)))},$$

where U is the activation energy, ν is the frequency of the vibrational mode associated with the interchange and $\beta = \frac{1}{\kappa_B T}$ is the Boltzmann's constant. Note that rescaling time one can set the term $\nu e^{-\beta U}$ to be 1. In a similar manner one can find the other exchange rates.

In the case of vacancy-driven diffusion we can use this mechanism regarding vacancies as being species of atoms. Based on this formalism, in the last part of Chapter 5 we shall derive the model for ordering in a binary alloy, with atoms exchanging places through vacancies. We also derive new equations by taking averages over the configurations.

Chapter 2

Mathematical background

2.1 Dynamical systems

In this section we introduce general tools and basic results of continuous dynamical systems theory which will be used frequently in the sequel; all the results are recalled without proof. The following definitions may be found in, among other sources, [4], [62], [64], [94].

Let X be a Banach space.

Definition 2.1 A family of evolution operators $\{S(t) : X \to X,\ t \geq 0\}$ is called a *(nonlinear) semigroup* on X if the following properties are satisfied:

(*i*) $S(0) = I$, the identity operator on X;

(*ii*) $S(t)(S(s)u) = S(t+s)u$, for all $u \in X$, for all $t, s \geq 0$;

(*iii*) the mapping $t \to S(t)u$ is continuous, for each $u \in X$;

(*iv*) $S(t)$ is a continuous (nonlinear) operator from X to itself, for all $t \geq 0$.

Furthermore, if we suppose that the Fréchet derivatives of $S(t)u$ in t exist up to order k and are continuous, then $\{S(t)\}_{t\geq 0}$ is said to be a C^k – semigroup.

The pair $\{X,\ S(t)\}$ is called a *semi-dynamical system.* If the operators $\{S(t)\}_{t>0}$ are one-to-one, then for all $t > 0$ there exists an inverse of $S(t)$, which we denote by $S(-t)$, and this operator maps $S(t)X$ onto X. We then get a family of

operators $\{S(t)\}_{t\in\mathbb{R}}$ satisfying $(i)\&(ii)$ on their domains of definition. In this case the pair $\{X, \{S(t), t \in \mathbb{R}\}\}$ is called a *dynamical system.*
The space X is often called *the phase space* (or *the state space*) and the map $S : \mathbb{R}_+ \times X \to X, \ (t, u_0) \mapsto S(t)u_0$ is called *a flow.*

Definition 2.2 The semigroup $\{S(t), t \geq 0\}$ is *completely continuous (uniformly compact)* for $t \geq t_0$ if

for all $\mathcal{B} \in X$, $\mathcal{B}$ bounded,

there exists $t_0 = t(\mathcal{B}) > 0$ such that $\bigcup_{t\geq t_0} S(t)\mathcal{B}$ is relatively compact in X.

We shall show in the next chapters that the equations we will consider are not completely continuous.

The most common way to define a continuous (semi-)dynamical system is by differential equations.

Example 2.3 Let us consider the following problem in a Banach space X:

$$\frac{du}{dt} + Au = f(u), \ \ t > 0 \tag{2.1.1}$$
$$u(0) = u_0 \in X,$$

with $f : X \to X$ is locally Lipschitz and A is a bounded operator in X. A function $u : [0, \ T) \to X$ is a *solution* of this problem on $[0, T)$ if u is continuous on $[0, T)$, continuously differentiable on $[0, T)$, $u(t) \in D(A)$ for $0 < t < T$, $u(0) = u_0$ and (2.1.1) is satisfied for all $t \in [0, T)$. We say that the problem is *well-posed* (see [84]), if there exists a solution $u(t; u_0)$ to the problem, the solution is unique, and depends continuously on u_0. Assume that for any initial condition $u_0 \in X$ the solution exists for any $t \geq 0$, then one can easily verify that

$$S(t)u_0 = u(t; u_0), \ \ t \geq 0$$

defines a continuous semi-dynamical system on X.

For any element $u_0 \in X$, we define the *positive semi-orbit* $\gamma^+(u_0)$ starting at u_0 as

$$\gamma^+(u_0) = \bigcup_{t\geq 0} S(t)u_0,$$

and similarly, when it exists, the *negative semi-orbit* $\gamma^-(u_0)$ ending at u_0 as

$$\gamma^-(u_0) = \bigcup_{t\leq 0}\{u(t)\},$$

where $u : (-\infty, 0] \to X$, such that $u(0) = u_0$ and for any $s \leq 0$, $S(t)u(s) = u(t+s)$, for $0 \leq t \leq -s$. The *complete orbit* through u_0 is the union of positive and negative orbits through u_0.

For any $u_0 \in X$ and for any set $B \subset X$, we define the *ω-limit set of u_0* (or B) and the *α-limit set of u_0* (or B) as

$$\omega(u_0) = \bigcap_{s\geq 0}\overline{\bigcup_{t\geq s} S(t)u_0}, \qquad \omega(B) = \bigcap_{s\geq 0}\overline{\bigcup_{t\geq s} S(t)B}$$

$$\alpha(u_0) = \bigcap_{s\leq 0}\overline{\bigcup_{t\leq s} S(-t)^{-1}u_0}, \qquad \alpha(B) = \bigcap_{s\leq 0}\overline{\bigcup_{t\leq s} S(-t)^{-1}B},$$

where the overbar means the closure in X.

A *stationary point*, or *equilibrium point* is a point $\phi \in X$ such that

$$S(t)\phi = \phi, \qquad \forall t \geq 0.$$

If $\{S(t)\}_{t\geq 0}$ is a C^1-semigroup, then an equilibrium point is called *hyperbolic* if the spectrum $\sigma(DS(t)(\phi))$ does not intersect the unit circle with center zero in $\mathbb{C}$, where $DS(t)$ is the derivative of $S(t)$.

If ϕ is a equilibrium point, then we can define the *stable* and *unstable manifolds of ϕ* as follows:

$$W^s(\phi) = \{u_0 \in X;\ S(t)u_0 \to \phi \text{ as } t \to \infty\}$$

$$W^u(\phi) = \{u_0 \in X;\ \text{there exists an orbit } u : (-\infty, 0] \to X \text{ such that}$$

$$u(0) = u_0 \text{ and } u(t) \to \phi \text{ as } t \to -\infty\}$$

A set $B \subset X$ is *positively invariant* (resp. *negatively invariant*) for the semigroup $S(t)$ if

$$S(t)B \subset B \qquad (\text{resp. } S(t)B \supset B), \qquad \forall t > 0.$$

The set B is called *invariant* for the semigroup $S(t)$ if $S(t)B = B, \quad \forall t \geq 0$.

A compact invariant set A is said to be a *maximal compact invariant set* if every compact invariant set of the semigroup is contained in A.

Definition 2.4 An invariant set $\tilde{\mathcal{A}} \in X$ is called an *attractor* if $\tilde{\mathcal{A}}$ possesses an open neighbourhood $\mathcal{U}$ such that, for every u_0 in $\mathcal{U}$ we have

$$\text{dist}(S(t)u_0,\, \tilde{\mathcal{A}}) \to 0, \text{ as } t \to \infty,$$

where 'dist' denotes the distance of a point to a set. The largest open set $\mathcal{U}$ that satisfies the above condition is called *the basin of attraction* of $\mathcal{A}$.

Definition 2.5 A set $\mathcal{A} \subset X$ is said to be the *global* (or *universal*) *attractor* for the semigroup $\{S(t),\, t \geq 0\}$ if the following conditions hold:

(i) $\mathcal{A}$ is a maximal compact invariant set in X,

(ii) $\mathcal{A}$ attracts bounded sets of X, i.e., for any bounded set $\mathcal{B} \subset X$ we have

$$\text{dist}(S(t)\mathcal{B},\, \mathcal{A}) \to 0, \text{ as } t \to \infty,$$

where here 'dist' represents the distance between two sets.

Related to the concept of attractor is the concept of absorbing sets.

Definition 2.6 We say that a subset $\mathcal{B} \subset X$ *absorbs bounded sets* of an open set $\mathcal{U} \supset \mathcal{B}$ (or $\mathcal{B}$ is *absorbing* in $\mathcal{U}$) if for any bounded set $\mathcal{B}_\mathcal{O} \subset \mathcal{U}$, there exists a time t_1 (depending upon $\mathcal{B}_\mathcal{O}$) such that

$$S(t)\mathcal{B}_\mathcal{O} \subset \mathcal{B}, \quad \forall t \geq t_1.$$

An important tool in studying of the stability of equilibrium solutions is a *Lyapunov function.*

Definition 2.7 A continuous function $V : X \to \mathbb{R}$ is called a *Lyapunov function* for the semigroup $\{S(t),\, t \geq 0\}$ if the following properties are satisfied:

(i) $V(x)$ is bounded below;

(ii) $V(x) \to \infty$ as $|x| \to \infty$;

(iii) $V(S(t)x)$ is nonincreasing in t for each x in X;

(iv) if x is such that $S(t)x$ is defined for $t \in \mathbb{R}$, and $V(S(t)x) = V(x)$, $\forall t \in \mathbb{R}$, then x is an equilibrium point.

Definition 2.8 A continuous semigroup $\{S(t),\, t \geq 0\}$ is said to be a *gradient system* if each bounded positive orbit is precompact and the system possesses a Lyapunov function.

For gradient systems we have the following results ([62]):

Proposition 2.9 *If $\{S(t),\, t \geq 0\}$ is a gradient system, then for all x in X the ω-limit set $\omega(x)$ is a subset of the set of equilibria.*

Proof. See [62], Lemma 3.8.2. □

Theorem 2.10 *If $\{S(t),\, t \geq 0\}$ is a gradient system, completely continuous, and the set of equilibria E is bounded, then there is a global attractor $\mathcal{A}$ for $S(t)$ and*

$$\mathcal{A} = \overline{W^u(E)} = cl\{z \in X;\ S(-t)z \text{ is defined for } t \geq 0 \text{ and } \operatorname{dist}(S(-t)z,\, E) \to 0 \text{ as } t \to \infty\}.$$

If X is a Banach space, then $\mathcal{A}$ is connected. If, in addition, each element of E is hyperbolic, then E is a finite set and

$$\mathcal{A} = \overline{\bigcup_{z \in E} W^u(z)}.$$

Proof. See [62], Theorem 3.8.5. □

As we shall see in the next chapters none of the nonlocal equations discussed there are gradient systems, and therefore we cannot apply Theorem 2.10.

Let $\mathcal{M}$ be an affine linear subspace of an infinite dimensional Hilbert space H (i.e., $\mathcal{M} = \overline{u} + \mathcal{M}_0$, with $\overline{u} \in H$ and $\mathcal{M}_0$ a linear subspace of H), $\mathcal{E} : \mathcal{M} \to \mathbb{R}$ a Gâteaux differentiable functional with respect to any direction in $\mathcal{M}_0$, and $u(t) \in \mathcal{M}$ for each t. The following two definitions can be also found in [44].

Definition 2.11 A *constrained gradient of $\mathcal{E}$ in H*, denoted by '$\operatorname{grad}_{\mathcal{M}}\mathcal{E}(u)$', is defined as an element of the closure $\overline{\mathcal{M}_0}$ of $\mathcal{M}_0$ in H such that for all $v \in \mathcal{M}$,

$$< \operatorname{grad}_{\mathcal{M}}\mathcal{E}(u), v >_H = \frac{d}{dh}\mathcal{E}(u + hv)|_{h=0}, \tag{2.1.2}$$

if such an element exists. Here $<,>$ represents the duality pairing in H.

Definition 2.12 A *constrained gradient flow* of $\mathcal{E}$ on $\mathcal{M}$ is defined by the equation:

$$\frac{\partial u(t)}{\partial t} = -K \operatorname{grad}_{\mathcal{M}} \mathcal{E}(u(t)), \tag{2.1.3}$$

for some positive constant K, called *the mobility*, which determines the rate at which u approaches equilibrium. Note that sometimes K may be replaced by a positive function.

Thus, the general principle for a gradient flow is that the dynamics of the system will have the property of reducing $\mathcal{E}$. Indeed, we have

$$\frac{d}{dt}\mathcal{E}(u(t)) = < \operatorname{grad}_{\mathcal{M}} \mathcal{E}(u(t)), \frac{\partial u}{\partial t}(t) > = -K \|\operatorname{grad}_{\mathcal{M}} \mathcal{E}(u(t))\|^2 \leq 0. \tag{2.1.4}$$

2.2 A mathematical overview of some macroscopic models for phase transitions in solids

The macroscopic models are models based on group dynamics. They are usually concerned with gross patterns and spatial scales. The matter is treated as being continuous, and the existence of atoms on a microscopic scale is not considered. At equilibrium the system can be characterized by a relatively small number of variables, e.g. density, volume, temperature, free energy, entropy. A state of a system described in this way may be referred to as a *macrostate*. Chemists make their observations in the macroscopic world and seek to understand the fundamental properties of matter at the level of the microscopic world (i.e. molecules and atoms). The macrostate of a system varies with time in two principal ways: by allowing heat to flow in, or doing work on the system. The general rules governing the macroscopic variables and their relations with other variables is the subject of thermodynamics. In this thesis we shall derive the kinetic equations for macroscopic models by postulating the evolution of a state as a gradient flow of a free energy functional. Motivated by this fact, we start with a discussion on the derivation of the free energy.

2.2.1 The free energy

In order to derive evolution equations for phase transitions in solids, such as ferromagnetic phase transition or phase separation in alloys, one does assume that the behaviour of the system can be described by a free energy functional which is defined as a function of an order parameter. We would expect that the system will evolve in such a way that its free energy decreases in time, a fact which is consistent with thermodynamic principles.

Let us consider a molten binary alloy which is confined to a bounded region $\Omega \in \mathbb{R}$ and, as in Section 1.2.1, let c_α and c_β be the concentrations of the two phases, α and β, respectively. We would like now to write the free energy of the mixture, such that the energy minimization argument will lead us to some law of evolution for the phase separation process. We take the order parameter to be the total solute atomic fraction in the alloy, defined by

$$u(x, t) = \frac{c_\alpha - c_\beta}{c_\alpha + c_\beta}. \tag{2.2.1}$$

Hence u is restricted to lie in the interval $[-1, 1]$, and $u \equiv 1$ in the pure α-phase and $u \equiv -1$ in the pure β-phase. For a $1:1$ composition we have $u \equiv 0$. We also note that (1.2.1) is satisfied, which imposes the mass conservation constraint (2.2.6). If we suppose that the interphase free energy of the two-phase mixture is neglected, then the free energy is the sum of the bulk free energies of the two components. Suppose that the domain Ω is situated on a lattice. Following Khachaturyan [68], if $F(c_\alpha)$ and $F(c_\beta)$ denote the specific free energies of each phase, and the system has N_α and N_β sites in the phases α and β, respectively, then the free energy at a given temperature T may be written as

$$E_0(u, T) = F(c_\alpha, T)N_\alpha + F(c_\beta, T)N_\beta.$$

The continuum analogue of this formula is

$$E_0(u, T) = \int_\Omega F(u(x), T)dx. \tag{2.2.2}$$

As we have discussed in Section 1.2.1, it was experimentally observed that at high temperatures the homogeneous state is a stable equilibrium, and for a temperature below a critical value T_c the equilibrium is a state with two coexisting

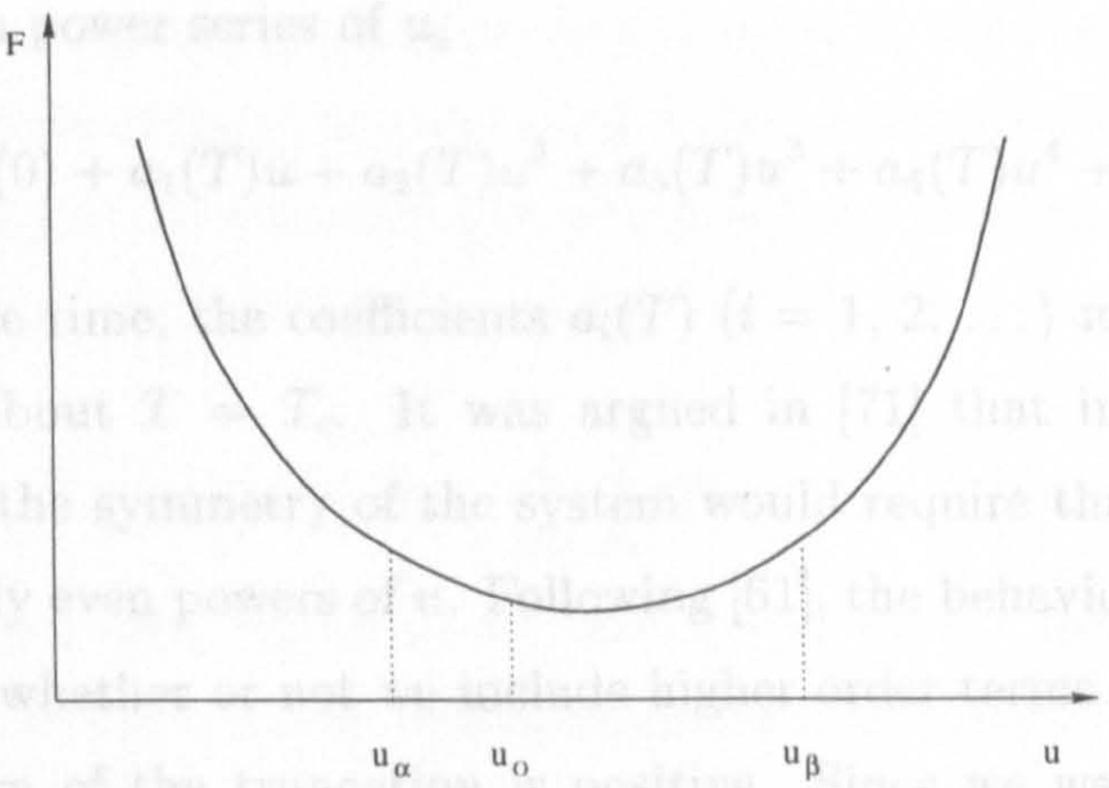

Figure 2.1: The bulk free energy $F(u)$ at some temperature $T > T_c$.

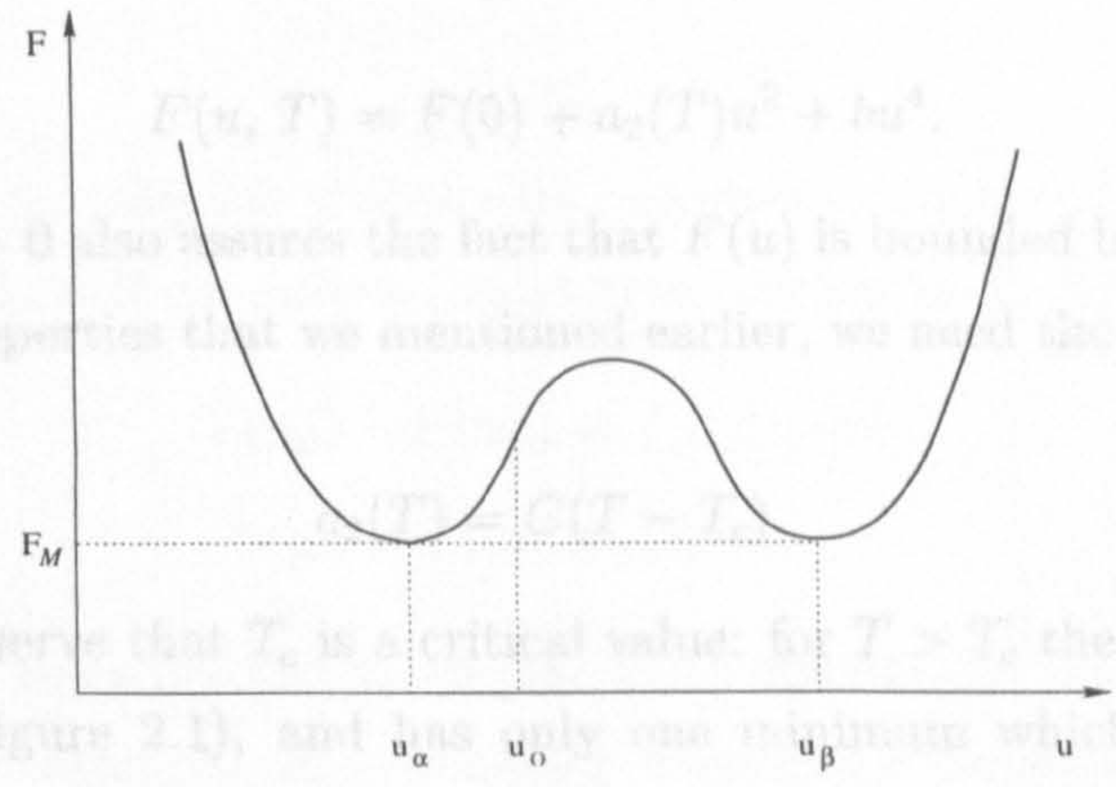

Figure 2.2: The bulk free energy $F(u)$ at some temperature $T < T_c$.

domains. We would like *the bulk free energy* $F(u, T)$ to be a convex function for $T > T_c$ (see Figure 2.1), and to be a double-well type function if $T < T_c$ (as shown in Figure 2.2), with two equal-depth symmetric minima. For $|u| > 1$, $F(u)$ is prolonged so that $F(u) \to \infty$ as $|u| \to \infty$. We shall see later that this choice for $F(u, T)$ agrees with experimental results.

In [70], Landau made the important assumption that in the vicinity of T_c the bulk free energy is an analytical function of order parameter (for the following discussion one can also consult [61], [71], [83], [89], [91] and [95]). Thus one can

expand $F(u, T)$ in power series of u,

$$F(u, T) = F(0) + a_1(T)u + a_2(T)u^2 + a_3(T)u^3 + a_4(T)u^4 + \dots, \qquad (2.2.3)$$

where, in the same time, the coefficients $a_i(T)$ $(i = 1, 2, \dots)$ may be expanded in Taylor series about $T = T_c$. It was argued in [71] that in the absence of an external field, the symmetry of the system would require that the expansion (2.2.3) contain only even powers of u. Following [61], the behaviour of the system is independent of whether or not we include higher order terms in the expansion if the leading term of the truncation is positive. Since we want the bulk free energy to be double-welled at low temperature, we suppose that $a_4(T) = b > 0$ and we shall consider the truncation of the Taylor expansion at the fourth order. We then have

$$F(u, T) = F(0) + a_2(T)u^2 + bu^4. \qquad (2.2.4)$$

The condition $b > 0$ also assures the fact that $F(u)$ is bounded below. If we want F to have the properties that we mentioned earlier, we need the coefficient $a_2(T)$ of the form

$$a_2(T) = C(T - T_c). \qquad (2.2.5)$$

We can easily observe that T_c is a critical value: for $T > T_c$ the bulk free energy is convex (see Figure 2.1), and has only one minimum which corresponds to the homogeneous phase $u \equiv 0$, while for temperatures below T_c, $F(u)$ becomes a double-well type function (see Figure 2.2), having two symmetric minima at $u = \pm(-a_2(T)/2b)^{1/2}$. These two solutions, which are denoted in Figure 2.2 by u_α and u_β, lead to the possibility that the mixture separates into two different phases. The region (u_α, u_β) is known as the *miscibility gap*, the region where F is concave is called the *spinodal region*, and its complementary region in the miscibility gap is known as the *metastable region*. For example, in the particular case $F(u) = \frac{1}{4}u^4 - \frac{1}{2}u^2$, these regions are: $(-1, 1)$, $(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$ and $(-1, -\frac{1}{\sqrt{3}}) \bigcup (\frac{1}{\sqrt{3}}, 1)$, respectively.

At all times, the concentration of each species contained in the vessel must remain constant, and this imposes the following constraint on the order parameter:

$$\frac{1}{|\Omega|}\int_\Omega u(x)dx = M > 0. \qquad (2.2.6)$$

It turns out that attempting to describe the dynamics of phase separation by considering gradient flows of $E_0(u)$ in a standard Hilbert space, constrained according to (2.2.6), will not give an evolution law which is both local and well-posed (see [44] and [45]). Taking the $L^2(\Omega)$ gradient flow of $E_0(u)$, one obtains the nonlocal equation

$$u_t = -f(u) + \frac{1}{|\Omega|}\int_\Omega f(u(y))dy, \tag{2.2.7}$$

where $f(u) = F'(u)$ (see Figure 2.3). One would expect the solution of this equation to evolve towards a state which minimizes the energy (2.2.2), subject to (2.2.6). If M lies in the interval (u_α, u_β), as in Figure 2.2, then it is well-known [20] that a solution of the minimization problem must be piecewise constant,

$$u(x) = \begin{cases} u_\alpha, & x \in S_1 \\ \\ u_\beta, & x \in S_2, \end{cases}$$

where S_1 and S_2 are disjoint measurable sets whose union is Ω, and u_α, u_β are defined by the *Maxwell conditions* (equal-area construction) (*cf.* Figure 2.3):

$$\begin{aligned} F(u_\beta) - F(u_\alpha) &= f_M(\beta - \alpha), \\ f(u_\alpha) &= f(u_\beta) = f_M. \end{aligned} \tag{2.2.8}$$

It turns out that equation (2.2.7) has far more equilibrium solutions which satisfy (2.2.6). For example, any bounded measurable function $u(x)$ satisfying $f(u) = const.$ is a steady state solution, regardless of whether $f(u) = f_M$ or not. Moreover, if $f'(u(x)) > 0$ *a.e.*, such solutions are linearly stable, without satisfying (2.2.8). These states are only local minimizers of the free energy (2.2.2).

The free energy $E_0(u)$ alone cannot predict the development of characteristic length scales with time, observed experimentally during phase separation. It was suggested [97] that the free energy at constant temperatures depends not only on the order parameter, but also on the order parameter gradient. Thus, additional terms must be considered in the free energy functional. We will therefore attempt to express the free energy as the sum of two contributions: one depending on the order parameter, and the other one depending on the order parameter derivatives. Let us denote by $\mathcal{F} = \mathcal{F}(u, \nabla u, \nabla^2 u, \dots)$ the free energy per unit volume (the specific free energy) and suppose that $\mathcal{F}$ is a smooth function of u

and its derivatives, such that we can expand this function in Taylor series about the uniform concentration $(\bar{u}, 0, 0, \dots)$. The total free energy over a volume Ω may be written as:

$$E(u) = \int_\Omega \mathcal{F}(u, \nabla u, \nabla^2 u, \dots) dx. \tag{2.2.9}$$

For small values of the gradient, the Taylor series expansion of $\mathcal{F}$ about $(\bar{u}, 0, 0, \dots)$ gives

$$\mathcal{F}(u, \nabla u, \nabla^2 u, \dots) = F(u) + \sum_{i=1}^{n} \frac{\partial \mathcal{F}}{\partial v_i} \frac{\partial u}{\partial x_i} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial \mathcal{F}}{\partial w_{ij}} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 \mathcal{F}}{\partial v_i \partial v_j} \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} + \mathcal{O}(3), \tag{2.2.10}$$

where $F(u) = \mathcal{F}(\bar{u}, 0, 0, \dots)$ is the bulk free energy per unit volume, and v_i, w_{ij} $(i, j = 1, 2, \dots)$ are the components of ∇u and $\nabla^2 u$, respectively.

Assuming the symmetry of the system to reflections $(x_i \to -x_i)$ and permutations $(x_i \to x_j)$ of axes (*isotropic medium*), we get that the partial derivatives of $\mathcal{F}$ with respect to v_i and w_{ij} are zero, apart from $\dfrac{\partial \mathcal{F}}{\partial w_{ii}}$ and $\dfrac{\partial^2 \mathcal{F}}{\partial v_i^2}$, which we shall denote by $\theta_1(u)$ and $\theta_2(u)$, respectively.

Thus, with these simplifying assumptions, we can approximate the total free energy free energy (2.2.9) by

$$E(u) = \int_\Omega \left\{ F(u) + \sum_{i=1}^{n} \left[\theta_1(u) \frac{\partial^2 u}{\partial x_i^2} + \theta_2(u) \left(\frac{\partial u}{\partial x_i} \right)^2 \right] \right\} dx. \tag{2.2.11}$$

Furthermore, by imposing the no-flux condition $\nabla u \cdot \mathbf{n} = 0$ on $\partial\Omega$, the application of the divergence theorem yields

$$\sum_{i=1}^{n} \int_\Omega \theta_1(u) \frac{\partial^2 u}{\partial x_i^2} \, dx = -\sum_{i=1}^{n} \int_\Omega \frac{\partial \theta_1(u)}{\partial u} \left(\frac{\partial u}{\partial x_i} \right)^2 dx.$$

Finally, neglecting the dependence of θ_1 and θ_2 on u and writing

$$\frac{\varepsilon^2}{2} := \theta_2(u) - \frac{\partial \theta_1(u)}{\partial u},$$

the expression of the free energy of the system enclosed in Ω reduces to

$$E_{GL}(u) = \int_\Omega [\frac{\varepsilon^2}{2} |\nabla u|^2 + F(u)] dx. \tag{2.2.12}$$

This theory is due to Cahn and Hilliard for metallic alloys (see [19]). An equivalent theory for magnetic domains is due to Landau and Ginzburg, and this is why (2.2.12) is often called the *Ginzburg-Landau free energy functional.* Based on this functional, with the constraint (2.2.6), Cahn and Hilliard derived in 1958 the related evolution equation, which is one of the leading models for the study of phase separation in isotropic binary alloys.

An inconvenient fact can appear here. For a very small scale of the microstructure (e.g., comparable to the atomic size) the gradient expansion of the free energy is no longer valid, and it was shown [66] that the Cahn-Hilliard approach fails to describe the evolution of the scale of the phase separation. In order to reproduce more faithfully the details of phase separation, two new directions are investigated. The first one involves considering mean field equations directly derived from the dynamic Ising model (a discussion on this approach will be made in Chapter 5). The other one, which we consider in the following two chapters, deals with a new free energy functional, in which the gradient term in (2.2.12) is replaced by a nonlocal term depending on the compositions at neighbouring points and vanishing when the concentration is constant. Instead of considering the Ginzburg-Landau free energy functional, we deal now with gradient flows of the following free energy functional:

$$E_K(u) = \frac{1}{4}\int_\Omega\int_\Omega \tilde{J}(|x-y|)(u(y)-u(x))^2\,dydx + \int_\Omega F(u(x))\,dx, \qquad (2.2.13)$$

where $\tilde{J}(\cdot) \in L^1(\Omega)$ is a kernel that measures interactions between particles at two different positions x and y, and it is assumed positive throughout this work. This functional has been initially proposed by van der Waals [97], and also considered by Khachaturyan in his book [68] (which is the reason for the subscript K).

In the remainder of this section, we will give an overview of some nonlinear evolutions which are used to model certain phase transition problems in materials science. We firstly present the Allen-Cahn model, which does not conserve the total mass of the order parameter, and we end with two conserving order parameter models, namely the viscous Cahn-Hilliard and the Novick-Cohen-Pego models.

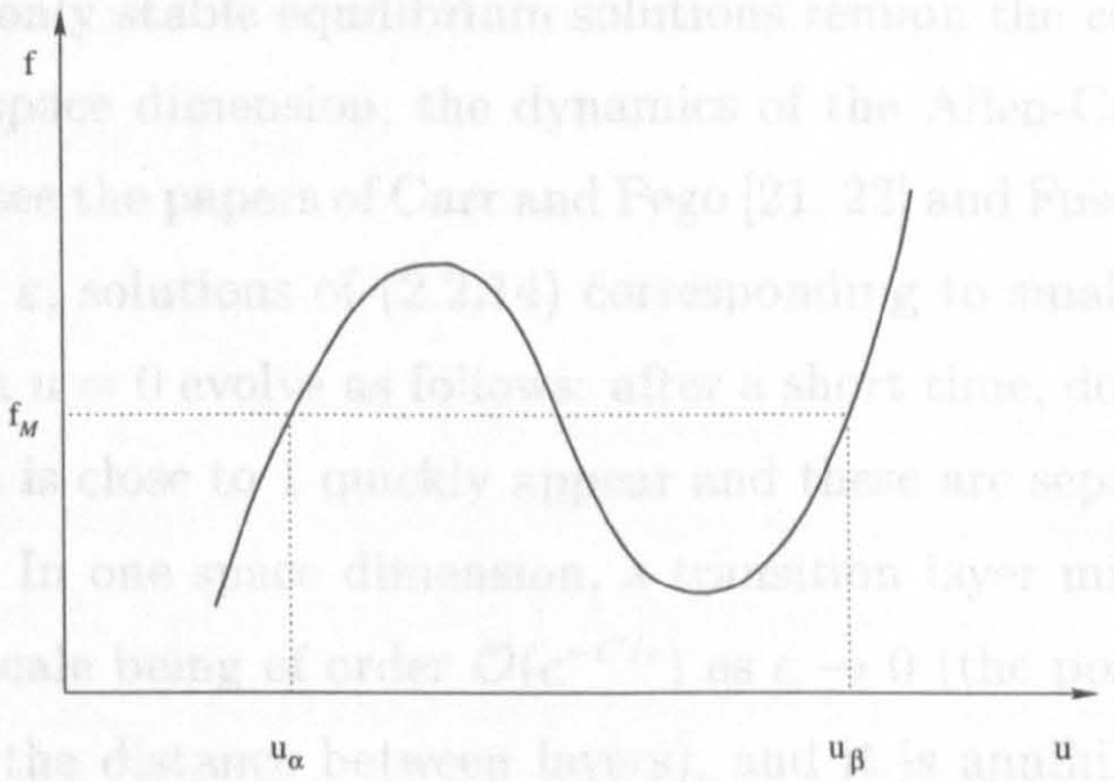

Figure 2.3: The bistable-type function $f(u)$.

2.2.2 The Allen-Cahn equation

The Allen-Cahn equation (also called the *bistable equation*) is an order parameter non-preserving model which can be used to model phase transitions in ferromagnetic materials [1], such as ferromagnetism. The equation for this model,

$$\frac{\partial u}{\partial t} = \varepsilon^2 \Delta u - f(u), \quad x \in \Omega,\ t > 0, \tag{2.2.14}$$

is derived as the $L^2(\Omega)$ gradient flow of the Ginzburg-Landau functional (2.2.12) for isotropic interfaces. Here $f(u) = F'(u)$ is of bistable type, as shown in Figure 2.3. The positive parameter ε measures the range of intermolecular forces in the system. The boundary conditions are usually taken to be

$$\nabla u \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega,\ t > 0.$$

Since the arguments depend only on the bistability property, we shall take for definiteness the usual choice for the function f, which is $f(u) = u^3 - u$. Note that this equation does not preserve the average value of the order parameter u.

When $\varepsilon = 0$, (2.2.14) is a simple ordinary differential equation, and the stable equilibrium solutions are either the constant functions $u \equiv \pm 1$, or the two phase solutions having $u(x) = -1$ for some $x \in \Omega$, and $u(x) = 1$ otherwise.

If $\varepsilon > 0$, then (2.2.14) is a second-order parabolic equation, for which the maximum principle, and consequently the comparison principle apply. If Ω is

convex, then the only stable equilibrium solutions remain the constant solutions $u \equiv \pm 1$. In one space dimension, the dynamics of the Allen-Cahn equation are well understood (see the papers of Carr and Pego [21, 22] and Fusco and Hale [53]). For small enough ε, solutions of (2.2.14) corresponding to small inhomogeneous perturbation from $u = 0$ evolve as follows: after a short time, domains where u is close to -1 and u is close to 1 quickly appear and these are separated by narrow transition layers. In one space dimension, a transition layer migrates extremely slowly, the time scale being of order $\mathcal{O}(e^{-C/\varepsilon})$ as $\varepsilon \to 0$ (the positive constant C depends only on the distance between layers), and it is annihilated by collision either with another layer or with the boundary. With probability one, solutions will then coarsen to either $u \equiv -1$ or $u \equiv 1$, depending on the initial data $u(x, 0)$. The latter statement is a straightforward consequence of the comparison principle. For more details on coarsening of solutions to (2.2.14) one can consult [21].

The Allen-Cahn equation defines a gradient flow in $L^2(\Omega)$, the Ginzburg-Landau free energy being the Lyapunov function, it possesses a global attractor which is compact, connected and is formed by equilibria and the orbits that connect them (see [23], [24], [62], [64]).

In the case of a quenched polycrystalline material, one can generalize (2.2.12) by considering the free energy as a function of many order parameters (u_1, u_2, ..., u_p). The domain-growth kinetics of the system can be described by a system of non-conserving order parameter equations which are similar to (2.2.14). Computer simulations for such a system were performed by Chen and Yang in [28], showing that the average domain radius grows as $t^{1/2}$ after a short transient following the quench, independent of the number of order parameters.

In Chapter 3 we shall derive the nonlocal non-conserving order parameter gradient flow using the free energy functional (2.2.13), and then compare some properties of solutions to that model with the solutions to the Allen-Cahn model. We find a stark contrast between the evolution of their corresponding solutions for small enough values of the rate parameters.

2.2.3 The viscous Cahn-Hilliard equation

The viscous Cahn-Hilliard equation,

$$(1-\alpha)u_t = \Delta(f(u) - \varepsilon^2\Delta u + \alpha u_t), \quad t > 0, \tag{2.2.15}$$

where $\alpha \in [0, 1]$, $f(u) = F'(u)$, was introduced by Novick-Cohen [80], who considered viscous effects in the Cahn-Hilliard model for phase separation in binary alloys which, as we can see later, is a limiting case of (2.2.15). The positive parameter ε has the same significance as in the previous subsection. This equation has been intensively studied by, among others, Bai *et al.* in [3], Elliott and Stuart [38], Grinfeld and Novick-Cohen [58], Novick-Cohen and Pego [82], and Temam [94]). If c_α and c_β, respectively, are the concentrations of the two components of the alloy, then $u(x, t)$ is defined by the formula (2.2.1), so $u \in [-1, 1]$.

On a bounded domain Ω, the equation (2.2.15) should be supplemented with boundary conditions on $\partial\Omega$. These are usually taken to be

$$\nabla u \cdot \mathbf{n} = \nabla(\varepsilon^2\Delta u - f(u)) \cdot \mathbf{n} = 0, \quad x \in \partial\Omega. \tag{2.2.16}$$

The first condition is the no-flux condition on the boundary, and the second one ensures that the total free energy of the mixture decreases in time. Using the first condition, we may simplify (2.2.16) and have

$$\nabla u \cdot \mathbf{n} = \nabla(\Delta u) \cdot \mathbf{n} = 0, \quad x \in \partial\Omega. \tag{2.2.17}$$

Using the translation $v = u - M$, we can rewrite (2.2.15) as

$$(1-\alpha)v_t = \Delta(f(v+M) - \varepsilon^2\Delta v + \alpha v_t), \quad t > 0, \quad \alpha \in [0, 1]. \tag{2.2.18}$$

For any mass $M \in [0, 1]$ and all $\alpha \in [0, 1]$, the equation (2.2.18) generates a semigroup on the space $H^1(\Omega) \bigcap \{L^2(\Omega);\ \int_\Omega u dx = 0\}$. Using ideas of [38], [62], [94], it is not hard to show that the viscous Cahn-Hilliard possesses a global attractor which is compact, connected and consists of equilibria and orbits connecting them. It has been proved in [13] and [59] that the semigroups are continuous in α, and in the limit $\alpha \to 0$ equation (2.2.15) reduces to the *Cahn-Hilliard equation*,

$$u_t = \Delta(f(u) - \varepsilon^2\Delta u), \tag{2.2.19}$$

and in the limit $\alpha \to 1$, (2.2.15) reduces to the *nonlocal reaction-diffusion equation*,

$$u_t = \varepsilon^2 \Delta u - f(u) + \int_\Omega f(u(x))dx, \tag{2.2.20}$$

proposed by Rubinstein and Sternberg [88], and also considered in [13].

The Cahn-Hilliard equation was initially derived by Cahn and Hilliard in [19], as a model for spinodal decomposition and coarsening (Ostwald ripening) phenomena in binary alloys. They derived this equation using physical concepts, such as generalized chemical potentials. It can also be derived as the $H^{-1}(\Omega)$ gradient flow of the Ginzburg-Landau functional (2.2.12) (see [44], [57]). The natural boundary conditions are (2.2.16) (or, equivalently, (2.2.17)), from which the mass conservation property (2.2.6) can be derived.

Existence and uniqueness theorems for solutions of (2.2.19) in appropriate functional space settings can be found in [39] and [94]; asymptotic behaviour of the solutions and stabilisation to equilibria have been proved in [103]. The semi-flow generated by the Cahn-Hilliard equation possesses a global attractor which is compact, connected and consists of equilibria and their connecting orbits (see [94]). In the one dimensional case it was shown that the equilibrium solutions are isolated [78] and the global attractor is finite dimensional, which is not the general case for higher space dimensions. Other discussions on the mathematical properties of the model can be also found in [34] for the bifurcation diagram, in [20], [58], [81], [100], [103] for the properties and the structure of equilibrium solutions when Ω is one-dimensional, in [77] for equilibria in higher space dimensions, in [57] and [75] for the spinodal decomposition in one dimension and, respectively, in higher dimensions, in [94] for the existence of inertial manifolds, in [7] for the spectral properties of solutions, in [2] for the extremely slowly evolving solutions in one space dimension, and [36] for numerical studies on the coarsening dynamics of solutions to (2.2.19).

The dynamics of the Cahn-Hilliard equation in one dimension for small ε may be described briefly as follows (for definiteness we consider $f(u) = u^3 - u$). If the mass M lies outside the miscibility gap $(-1, 1)$, then all solutions decay to the trivial solution $u \equiv M$ (see [39], [103]). If M lies in the miscibility gap, then

after an initial transient period the solution takes the form of a finite number of transition layers separated by regions where u is alternatively -1 or $+1$. These transition layers will migrate slowly relative to one another and the smaller scale layers will be annihilated (the coarsening process takes place). Asymptotically, solutions approach a stable stationary solution which is a global minimizer of the free energy (2.2.12). In [20] it has been proved that the stable equilibrium solutions have to be monotone.

If ε or $|M|$ is big enough, then there is a unique global solution which decays to the constant mass M as $t \to \infty$ (see [39]).

The nonlocal reaction-diffusion equation (2.2.20) was also used to model the phase separation process in binary mixtures which preserve the total mass of the two components, but it does not have the pattern formation capabilities of (2.2.19). It can been derived as the $L^2(\Omega)$ constrained (mass-conserving) gradient flow of the Ginzburg-Landau functional (2.2.12) or, alternatively, by adding a nonlocal term to the Allen-Cahn equation, which makes the total mass of u to be a conserved quantity, i.e., such that (2.2.6) is satisfied. This is why (2.2.20) is sometimes referred to as the *nonlocal Allen-Cahn equation.* We shall not use this name for (2.2.20) in this work, since we are going to use it later for a different equation. Rubinstein and Sternberg [88] have studied the behaviour of the solution of (2.2.20) with Neumann boundary conditions. They used multiple time-scale asymptotic expansions, and formally obtained that the domain Ω is divided in regions where the order parameter u is close to the local minima of $F(u)$. Based on energy methods combined with some a priori estimates, L. Bronsard and B. Stoth [13] studied the asymptotic behaviour of radially symmetric solutions of (2.2.20).

In Chapter 4 we shall introduce and discuss some nonlocal versions of these equations.

2.2.4 The Novick-Cohen-Pego equation

As mentioned in [44], the gradient flows of (2.2.2) with respect to $L^2(\Omega)$, or $H^{-1}(\Omega)$, or any other standard Hilbert space will not give a local evolution law. Starting from the free energy (2.2.2), one can get a well-posed local equation when a different type of approach is used. In [82], Novick-Cohen and Pego have considered gradient flows of (2.2.2) with respect to the following Hilbert space

$$X = \{u \in L^2(\Omega); \int_\Omega u(x)dx = 0\}. \tag{2.2.21}$$

They defined for some $\nu > 0$ the operator

$$Au = (\nu\Delta - I)^{-1}\Delta u, \tag{2.2.22}$$

and used the following inner product in X:

$$\langle u, v\rangle_X = \langle A^{-1}u, v\rangle_{L^2}.$$

The mass-conserving gradient flow of (2.2.2) with respect to this inner product is

$$u_t = \Delta(f(u) + \nu u_t), \tag{2.2.23}$$

where $f(u) = F'(u)$.

They proved global existence in $L^\infty(\Omega)$ of solutions for $t > 0$ by exhibiting a positively invariant interval for u, and the stabilisation of these solutions to a steady state solution. In this case the set of equilibria turns out to be richer that the corresponding set of the Cahn-Hilliard equation; it also contains steady states which satisfy $f(u) = 0$, regardless of whether u is a global minimum for (2.2.2) or not. The constant solutions are unstable in the spinodal region, as for the Cahn-Hilliard equation, but their dispersion relation does not identify a preferred wave number with maximal growth rate. As we shall see in the next chapter, Section 3.6, this equation can be derived in a rather different way, by considering Padé approximations obtained from the gradient expansion of $E_K(u)$.

Chapter 3

The nonlocal Allen-Cahn equation

3.1 Introduction

This chapter is devoted to the following equation,

$$u_t = \frac{\gamma}{\varepsilon}\int_\Omega J(\frac{|x-y|}{\varepsilon})(u(y)-u(x))\,dy - f(u),\ x\in\Omega,\ t>0, \tag{3.1.1}$$

where Ω is a convex bounded domain in $\mathbb{R}$, $u(x,t)$ is the order parameter representing the state at position x and time t, $J(\cdot)$ is an $L^1(\mathbb{R})$ kernel, $f(u)$ is a (dissipative) bistable nonlinearity, and γ and ε are positive constants. This equation is subject to the initial condition

$$u(x,0) = u_0(x). \tag{3.1.2}$$

As we shall see later, no boundary conditions are required.

The equation (3.1.1) may model a variety of physical and biological phenomena involving media with properties varying in space. We may regard this equation as the nonlocal version of the Allen-Cahn equation (2.2.14) because, as one can observe, to determine the evolution of $u(x,t)$ in time we need to take into account the values of the state in a neighbourhood of the site x. Equation (3.1.1)

has been introduced by Bates, Fife and co-workers. In particular, the paper [42] sets out the general theory of these (integro-differential) equations and gives an overview of known results. Bates and Chmaj [5] give a careful derivation of the equation directly from the Ising model and describe steady state solutions. In [43] Fife establishes the existence of a spatially nonuniform stationary solution on the real line connecting two uniform states. Monotone travelling waves and stationary waves in one-dimensional case were studied in [9]. In [29] Chen found an infinite number of non-monotone discontinuous waves, and Bates and Chmaj analyse in [6] the discrete version of this equation. The bulk of Sections 3.4 and 3.5 is contained in [32].

We begin with a brief derivation of the Khachaturyan free energy functional, and based on this functional we derive an L^2-gradient flow. The equation (3.1.1) is obtained as the restriction of this gradient flow to Ω. Concerning this equation we show the well-posedness in $L^\infty(\Omega)$ (with Ω bounded in $\mathbb{R}$), and examine some properties of the stationary solutions in the special case $J \equiv 1$, properties that will be used in the following sections. The main results of this chapter are related to coarsening of solutions to (3.1.1)+(3.1.2) when $J(\cdot) \geq 0$, and the approximation of the generated flow by flows obtained using a Padé approximation scheme. We prove the non-coarsening property of a solution starting from initial data that change sign, the key tool in the proof being the comparison principle that (3.1.1) obeys. In Section 3.7 we outline a numerical approximation method and show runs to illustrate the result of the Section 3.5. We end this chapter with some comments on the similarities and differences between this equation and the Allen-Cahn equation.

3.2 Derivation of the equation

Let us consider a binary alloy on a 1-dimensional lattice Λ, such that the sites are occupied by atoms of two species A or B. To each lattice site k we assign a spin variable $\sigma(k)$ which can take only values, $\sigma(k) = 1$ if the site is occupied by an A-atom, and $\sigma(k) = -1$ for a B-atom. Denote by $p(k)$ the probability of

an A-atom at site k. We denote by $u(k)$ the average value of this spin, which is given by

$$u(k) = \mathbf{E}(\sigma(k)) = 2p(k) - 1.$$

Let $\tilde{J}(|k-k'|)$ be the energy of interactions between particles at positions k and k' (which is considered nonnegative throughout this thesis), and $F(u)$ be the bulk free energy of the system. The function $F(u)$ has a double-well form as in Figure 2.2, and we suppose that it has two equal depth minima at $u \equiv \pm 1$. Then the Helmholtz free energy of this discrete system, derived by Bates and Chmaj [5], [6] (see also [68]), is

$$E(u) = \frac{1}{4} \sum_{k,k' \in \Lambda} \tilde{J}(|k-k'|)(u(k)-u(k'))^2 + \sum_{k \in \Lambda} F(u(k)). \tag{3.2.1}$$

If the lattice Λ covers the whole space $\mathbb{R}$, then the expression of the energy (3.2.1) in the continuum mean-field approximation is:

$$E_K(u) = \frac{1}{4} \int_{\mathbb{R}} \int_{\mathbb{R}} \tilde{J}(|x-y|)(u(y)-u(x))^2 \, dydx + \int_{\mathbb{R}} F(u(x)) \, dx. \tag{3.2.2}$$

If in (3.2.2) we take

$$\gamma = \int_{\mathbb{R}} \tilde{J}(|r|)dr > 0 \quad \text{and} \quad J(r) = \frac{1}{\gamma}\tilde{J}(r),$$

we get

$$E_K(u) = \frac{\gamma}{4} \int_{\mathbb{R}} \int_{\mathbb{R}} J(|x-y|)(u(y)-u(x))^2 \, dydx + \int_{\mathbb{R}} F(u(x)) \, dx, \tag{3.2.3}$$

where now

$$\int_{\mathbb{R}} J(|r|)dr = 1.$$

Note that this normalisation condition enables us to view the nonlocal term in (3.2.3) as being a weighted average of the values of $(u(y)-u(x))^2$ over all sites in the lattice. The parameter γ can be regarded as a convenient measure of the overall strength of interactions between particles at lattice sites x and y. We would like now to derive the $L^2(\mathbb{R})$ gradient flow of (3.2.3). We denote here, and throughout this work, by $< \cdot, \cdot >$ and $\| \cdot \|$ the L^2-inner product and the L^2-norm, respectively.

We need firstly the gradient of $E_K(u)$ in $L^2(\mathbb{R})$. This is an element of $L^2(\mathbb{R})$, denoted by $\frac{\delta E_K}{\delta u}(u)$, which satisfies

$$\frac{d}{dh}E_K(u+hv)|_{h=0} = < \frac{\delta E_K}{\delta u}(u), v >, \quad \text{for all } v \in L^2(\mathbb{R}).$$

We use Definition 2.11, with $\mathcal{M} = H = L^2(\mathbb{R})$. For all $v \in L^2(\mathbb{R})$, we have successively:

$$\begin{aligned}
&\frac{d}{dh}E_K(u+hv)|_{h=0} = \\
&= \frac{\gamma}{4}\frac{d}{dh}\left\{\int_{\mathbb{R}}\int_{\mathbb{R}} J(|x-y|)[u(x)+hv(x)-u(y)-hv(y)]^2 dxdy\right\}_{h=0} \\
&\quad + \frac{d}{dh}\left\{\int_{\mathbb{R}} F(u(x)+hv(x))dx\right\}_{h=0} \\
&= \frac{\gamma}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} J(|x-y|)(u(x)-u(y))(v(x)-v(y))dxdy + \int_{\mathbb{R}} F'(u(x))v(x)dx \\
&= \frac{\gamma}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} J(|x-y|)[u(x)v(x)+u(y)v(y)-u(x)v(y)-u(y)v(x)]dxdy + \\
&\quad + \int_{\mathbb{R}} f(u(x))v(x)dx \\
&= \gamma\int_{\mathbb{R}}\int_{\mathbb{R}} J(|x-y|)[u(x)v(x)-u(y)v(x)]dxdy + \int_{\mathbb{R}} f(u(x))v(x)dx \\
&= < \gamma\int_{\mathbb{R}} J(|x-y|)[u(x)-u(y)]dy + f(u),\ v >, \qquad (3.2.4)
\end{aligned}$$

with $f(u) = F'(u)$ (see Figure 2.3). By the above definition, the gradient of (3.2.3) in $L^2(\mathbb{R})$ is represented by

$$\frac{\delta E_K}{\delta u}(u) = \gamma\int_{\mathbb{R}} J(|x-y|)[u(x)-u(y)]dy + f(u(x)).$$

Consequently, the $L^2(\mathbb{R})$ gradient flow is

$$u_t = \gamma\int_{\mathbb{R}} J(|x-y|)[u(y)-u(x)]\,dy - f(u), \quad x \in \mathbb{R}. \qquad (3.2.5)$$

By changing the variable under the integral to $\eta = y - x$, and then rescaling the space by a positive constant ε, we can rewrite (3.2.5) as

$$u_t = \gamma\int_{\mathbb{R}} J(|\eta|)[u(x+\varepsilon\eta)-u(x)]\,d\eta - f(u), \quad x \in \mathbb{R}. \qquad (3.2.6)$$

We now change the variable by taking $y = x + \epsilon\eta$, and obtain

$$u_t = \frac{\gamma}{\varepsilon}\int_{\mathbb{R}} J(\frac{|x-y|}{\varepsilon})[u(y)-u(x)]dy - f(u), \quad x \in \mathbb{R}, \qquad (3.2.7)$$

which is the $L^2(\mathbb{R})$ gradient flow of the rescaled energy

$$\mathcal{E}_K(u) = \frac{\gamma}{4\varepsilon}\int_{\mathbb{R}}\int_{\mathbb{R}} J(\frac{|x-y|}{\varepsilon})[u(y)-u(x)]^2\,dydx + \int_{\mathbb{R}} F(u(x))\,dx. \qquad (3.2.8)$$

3.3 The semigroup approach

In this section we restrict ourselves to a convex bounded domain $\Omega \subset \mathbb{R}$. We would like to show that (3.2.7) generates a dynamical system on $X = L^\infty(\Omega)$. In fact (3.2.7) generates a dynamical system in various function spaces (e.g. $L^2(\Omega)$, $C(\Omega)$ etc.), but the $L^\infty(\Omega)$ setting is the best choice for the properties that we are going to prove in the next sections of this chapter. We consider the following assumptions on J and f:

$(\mathcal{H}_1)$ $\quad J \in L^1(\mathbb{R}),\ \ J(\cdot) \geq 0,\ \ \int_{\mathbb{R}} J(|x|)dx = 1,$

$(\mathcal{H}_2)$ $\quad f \in C^1(\Omega)$ is a function of bistable type (as shown in Figure 2.3), i.e., it has exactly three zeros at z_{-1}, z_0 and z_1, with $f'(z_{\pm 1}) > 0,\ \ f'(z_0) < 0$.

We write the equation (3.2.7) on the bounded domain Ω as

$$u_t = \gamma\int_\Omega J_\epsilon(|x-y|)[u(y)-u(x)]dy - f(u),\quad x \in \Omega, \qquad (3.3.1)$$

where by J_ε we denote

$$J_\epsilon(x) = \frac{1}{\varepsilon}J(\frac{x}{\varepsilon}). \qquad (3.3.2)$$

Setting

$$A_\epsilon u(x) = \int_\Omega J_\epsilon(|x-y|)[u(y)-u(x)]dy, \qquad (3.3.3)$$

we can write (3.2.7) in the abstract form:

$$\frac{\partial u}{\partial t} = \gamma A_\epsilon u - f(u),\quad t > 0. \qquad (3.3.4)$$

In what follows we shall establish that equation (3.3.4) with initial data

$$u(x,0) = u_0(x),\quad x \in \Omega, \qquad (3.3.5)$$

is well-posed for u_0 in $L^\infty(\Omega)$.

Definition 3.1 We define a *solution* for the problem (3.3.4)+(3.3.5) on an interval $[0,T)$ to be a continuous function $u : [0,T) \to L^\infty(\Omega)$, differentiable on $(0,T)$, such that $f(u(\cdot)) : [0,T) \to L^\infty(\Omega)$ is continuous, u satisfies (3.3.4) on $(0,T)$ and $u(0) = u_0$.

We start with the following two lemmas:

Lemma 3.2 *The operator A_ε is bounded on $L^\infty(\Omega)$.*

Proof. Indeed, for all $x \in \Omega$ we have

$$\begin{aligned}
|A_\varepsilon u(x)| &= |\int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))dy| \\
&\le \int_\Omega J_\varepsilon(|x-y|)(\operatorname{ess\,sup}_{y\in\Omega}|u(y)| + \operatorname{ess\,sup}_{x\in\Omega}|u(x)|)dy \\
&\le 2\left(\int_\Omega J_\varepsilon(|x-y|)dy\right)\|u\|_\infty \\
&\le 2\left(\int_{\mathbb{R}} J_\varepsilon(|x-y|)dy\right)\|u\|_\infty \\
&= 2\|u\|_\infty,
\end{aligned}$$

which implies the boundedness of A_ε in the L^∞-norm. □

Lemma 3.3 *If f is locally Lipschitz and satisfies the following property*

$$\liminf_{|s|\to\infty} \frac{f(s)}{s} \ge 0, \tag{3.3.6}$$

then the problem

$$\frac{dw}{dt} = -f(w), \;\; w(0) = \xi \tag{3.3.7}$$

has a unique global solution $w \in C^1([0,\infty))$.

Proof. For any $\mu > 0$, the hypothesis (3.3.6) implies that

$$-f(s)s \le C_\mu - \mu s^2, \quad \text{for all } s \in \mathbb{R}, \tag{3.3.8}$$

where C_μ is a positive constant depending on μ. Existence theory for ordinary differential equations yields a unique local solution $w(t)$ such that

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}w^2(t) &= -f(w(t))w(t) \\
&\le C_\mu - \mu\, w^2(t), \quad \text{for all } t \ge 0,
\end{aligned}$$

which, after integration, implies that

$$w^2(t) \leq w^2(0)\exp(-2\mu t) + \frac{C_\mu}{\mu}(1-\exp(-2\mu t))$$
$$\leq \max(\xi^2, \frac{C_\mu}{\mu}), \quad \text{for all } t \geq 0.$$

Hence, a unique global solution exists. □

Theorem 3.4 (local existence) *Suppose J satisfies the conditions $(\mathcal{H}_1)$, f is locally Lipschitz, and $u_0 \in L^\infty(\Omega)$. Then there exists $T = T(u_0) > 0$ such that the problem (3.3.1)+(3.3.5) has a unique local solution $u \in C^1([0, T), L^\infty(\Omega))$. If f is C^k, $1 \leq k \leq \infty$, then $u \in C^{k+1}([0, T), L^\infty(\Omega))$.*

Proof. Since A_ε is bounded on $L^\infty(\Omega)$, the right hand side of (3.3.4) is a locally Lipschitz perturbation of a bounded operator on the Banach space $L^\infty(\Omega)$. We then have the existence and uniqueness of a local solution on a maximal interval of existence $[0, T)$. (See, for example, [64] Theorem 3.3.3.). □

For the evolution governed by (3.3.1) P. C. Fife [42] showed that a maximum principle holds, as well as a comparison principle. For these principles to hold the condition $J(\cdot) \geq 0$ is essential. We give here an adapted version of the comparison principle presented in [42].

Lemma 3.5 *Let u_0, $v_0 \in L^\infty(\Omega)$ satisfying $u_0(x) \leq v_0(x)$ a.e. in Ω. If $u(x, u_0)$ and $u(x, v_0)$ are the solutions to (3.3.4) + (3.3.5) starting from u_0 and v_0, respectively, then*

$$u(x, u_0) \leq u(x, v_0), \quad \text{a.e. in } \Omega, \quad \text{for all } t \in [0, \infty).$$

Proof. This is an immediate consequence of Prop. B, [42]. □

Remark 3.6 In Section 3.5, we shall prove (see Prop. 3.27) the comparison principle for equation (3.3.4) with A_ε replaced by a more general operator.

Using the result of Lemma 3.5, we can now prove the following theorem:

Theorem 3.7 (global existence) *Suppose the hypotheses of Theorem 3.4 are fulfilled and, moreover, f satisfies the additional condition (3.3.6). Then there exists a global solution to (3.3.1)+(3.3.5) such that $u \in C^1([0, \infty), L^\infty(\Omega))$. For all $T > 0$, the mapping $u_0 \mapsto u$ is Lipschitz continuous from $L^\infty(\Omega)$ into $C([0, T), L^\infty(\Omega))$.*

Proof. Theorem 3.4 guarantees the existence and uniqueness of a local solution. In order to show that this solution is globally defined, one needs to prove the boundedness of the solution. We start with an initial data u_0 that satisfies

$$a \leq u_0(x) \leq b, \quad a.e. x \in \Omega.$$

We then consider the solutions $w_a(t)$ and $w_b(t)$ to (3.3.7) with initial data $w(0) = a$ and $w(0) = b$, respectively. We observe that these functions also verify (3.3.4), and by the comparison principle stated in Lemma 3.5 we get

$$w_a(t) \leq u(x, t; u_0) \leq w_b(t), \quad \text{for all } t > 0.$$

Since $w_a(t)$ and $w_b(t)$ are bounded, the solution $u(x, t; u_0)$ is locally bounded, and, hence, a unique global solution exists.

The Lipschitz continuity of the map $u_0 \mapsto u$ is a consequence of the following argument. For an arbitrary fixed $T > 0$, let u and v be the $C^1([0, T), L^\infty(\Omega))$ solutions starting from initial data u_0 and, respectively, v_0, with $u_0, v_0 \in L^\infty(\Omega)$. Then we have

$$u_t(t) - v_t(t) = \gamma A_\epsilon(u(t) - v(t)) + f(v(t)) - f(u(t)), \text{ for all } 0 \leq t < T.$$

Multiplying the above relation by $u(t) - v(t)$, and using the boundedness of A_ϵ and the local Lipschitz continuity of f, we get

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}|u(t) - v(t)|^2 &\leq 2\gamma\|u(t) - v(t)\|_\infty^2 + L(T)\|u(t) - v(t)\|_\infty^2 \\ &= (2\gamma + L(T))\|u(t) - v(t)\|_\infty^2, \end{aligned}$$

and therefore

$$\|u(t) - v(t)\|_\infty \leq e^{2T(2\gamma + L(T))}\|u_0 - v_0\|_\infty,$$

which yields the Lipschitz continuity of the map $u_0 \mapsto u$. □

Remark 3.8 An immediate consequence of Theorem 3.4 is the existence of a continuous semigroup on $L^\infty(\Omega)$ defined by the family of solution operators $\{T(t),\, t \geq 0\}$, with $T(t)u_0 \stackrel{def}{=} u(t;\, u_0)$. Since the operator A_ε is bounded on $L^\infty(\Omega)$, for all $\varepsilon > 0$, we may as well construct a unique local solution for backward time, defined on a maximal interval, say $(-T,\, 0]$. We thus get a flow defined on $L^\infty(\Omega)$, and so the problem (3.3.4) + (3.3.5) generates a dynamical system in $L^\infty(\Omega)$. Under some restrictive conditions on f (e.g. f is bounded) one can extend the solution on $(-T,\, 0]$ to a global one defined on the negative semi-axis.

Remark 3.9 One can easily check that

$$\mathcal{L}(u) = \frac{\gamma}{4}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))^2\, dydx + \int_\Omega F(u(x))\, dx. \qquad (3.3.9)$$

is a Lyapunov functional for the semigroup $\{T(t),\, t \geq 0\}$. Indeed, since $J(\cdot) \geq 0$ and $F(u)$ is bounded below (being a double-well type function), the functional $\mathcal{L}(u)$ is bounded below as well. We also have that

$$\mathcal{L}(u) \to +\infty, \quad \text{as } \|u\|_2 \to +\infty,$$

and

$$\frac{d}{dt}\mathcal{L}(T(t)u_0) = -\|u_t\|_2^2 \leq 0, \qquad (3.3.10)$$

where the equality holds if u is an equilibrium solution for (3.3.1).

Remark 3.10 If we take $f(u) = u^3 - u$, which satisfies the assumption (3.3.6), and $-1 \leq u(x,\, 0) \leq 1,\ x \in \Omega$, then from the comparison principle (Lemma 3.5) we get the *a priori* bound

$$-1 \leq u(x,\, t) \leq 1,\ \ x \in \Omega,\ \text{for all } t > 0.$$

Indeed, if we take $u_0(x) = u(x,\, 0),\, x \in \Omega$ in Lemma 3.5, and $v_0 \equiv 1$, then $u(x,\, t) \leq 1,\, x \in \Omega$, for all $t > 0$. Similarly, we take $u_0 \equiv -1$ and $v_0(x) = u(x,\, 0),\, x \in \Omega$, and get $-1 \leq u(x,\, t),\ x \in \Omega,\ \text{for all } t > 0$.

For essentially bounded initial data, we may prove the following result for the solutions of (3.3.1).

Proposition 3.11 *Let $u_0 \in L^\infty(\Omega)$ and suppose that f is as in Theorem 3.7. If $u(x, t)$ denotes the global solution of (3.3.1)+(3.3.5), then we have*

$$\|u_t(\cdot, t)\|_2 \longrightarrow 0, \qquad as \quad t \longrightarrow \infty. \tag{3.3.11}$$

Proof. Using (3.3.10) and the fact that $\mathcal{L}(u)$ is a Lyapunov functional for the semigroup generated by (3.3.1), we find two constants C_1, C_2 (which are independent of t) such that

$$C_1 \leq \mathcal{L}(u(x,t)) \leq \mathcal{L}(u_0(x)) \leq C_2, \quad \forall\, t \geq 0. \tag{3.3.12}$$

Integrating (3.3.10) with respect to time and using (3.3.12), results in

$$\int_0^\infty \|u_t(\cdot, t)\|_2^2 \, dt \leq C < +\infty, \quad \forall\, t \geq 0, \tag{3.3.13}$$

from which the convergence (3.3.11) follows if we manage to prove that the function $h(t) := \|u_t(\cdot, t)\|_2^2$ is uniformly continuous for all $t \in [0, \infty)$. From Theorem 3.7 we get that $u(\cdot, t)$ is uniformly bounded in the L^∞-norm. Hence from (3.3.1) and the boundedness of $\|A_\varepsilon\|_\infty$ we obtain the uniform boundedness of $\|u_t(\cdot, t)\|_\infty$. Using the fact that f is locally Lipschitz and A_ε is bounded on $L^\infty(\Omega)$, then for all $t > s \geq 0$ we have:

$$\begin{aligned}
|h(t) - h(s)| &= \Big| \int_\Omega [u_t^2(x,t) - u_t^2(x,s)]\, dx \Big| \\
&\leq \int_\Omega |u_t(x,t) + u_t(x,s)||u_t(x,t) - u_t(x,s))|\, dx \\
&\leq C_1 \int_\Omega |u_t(x,t) - u_t(x,s)|\, dx \qquad (\text{since } \|u_t(\cdot, t)\|_\infty < \infty) \\
&= C_1\gamma \int_\Omega |A_\varepsilon(u(x,t) - u(x,s)) - f(u(x,t)) + f(u(x,s))|\, dx \\
&\leq C_1\gamma \int_\Omega |A_\varepsilon(u(x,t) - u(x,s))|\, dx + C_1 \int_\Omega \|f(u(t)) - f(u(s))\|_\infty\, dx \\
&\leq 2C_1\gamma \|u(t) - u(s)\|_\infty + C_1 L_\Omega \|u(t) - u(s)\|_\infty \\
&\qquad (\text{since } A_\varepsilon \text{ is bounded on } L^\infty(\Omega) \text{ and } f \text{ is locally Lipschitz}) \\
&\leq C|t - s| \qquad (\text{since } t \mapsto u(\cdot, t) \text{ is } C^1 \text{ on } [s, t], \text{ and } \|u_t\|_\infty < \infty).
\end{aligned}$$

This shows that $h(t)$ is uniformly Lipschitz, thus the proof is complete. □

3.4 Stationary solutions

A stationary solution $u \in L^\infty(\Omega)$ is an extreme value of the free energy functional (3.2.8), that is,

$$u \in L^\infty(\Omega), \text{ such that } \frac{d}{dh}\mathcal{E}_K(u+hv)|_{h=0} = 0, \text{ for all } v \in L^\infty(\Omega).$$

Thus, the equilibrium solutions are solutions of the equation

$$\gamma \int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))dy - f(u(x)) = 0, \quad x \in \Omega. \tag{3.4.1}$$

The existence and stability of the solutions to (3.4.1) (with $J_\varepsilon = J$) have been studied by Bates and Chmaj [5], in both cases $J(\cdot) > 0$ and J changes sign. We start with the following lemma:

Lemma 3.12 *If f satisfies the assumption (3.3.6), then for all $\gamma \geq 0$ the set of equilibria is bounded in $L^\infty(\Omega)$.*

Proof. Multiplying (3.4.1) by u and using the inequality $(a-b)b \leq a^2$, we get

$$\begin{aligned} f(u(x))u(x) &= \gamma \int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))u(x)dy \\ &\leq \gamma \int_\Omega J_\varepsilon(|x-y|)u^2(y)dy \\ &\leq \gamma \|u\|_\infty^2, \quad \text{for almost all } x \in \Omega. \end{aligned} \tag{3.4.2}$$

On the other hand, by choosing $\mu = \gamma + 1$ in (3.3.8), we have

$$(\gamma+1)|u(x)|^2 - C_\gamma \leq f(u(x))u(x),$$

which combined with (3.4.2) gives

$$(\gamma+1)|u(x)|^2 - C_\gamma \leq \gamma \|u\|_\infty^2, \quad \text{for all } x \in \Omega,$$

with C_γ a positive constant. By passing to the supremum in the left-hand side of the last inequality yields the $L^\infty(\Omega)$ boundedness of u. □

For definiteness, we shall take $f(u) = u^3 - u$ in the remaining sections of this chapter; however, the arguments below can be easily adapted to deal with any bistable nonlinearity.

In the particular case $\gamma = 0$, the equation (3.4.1) reduces to

$$f(u(x)) = 0, \quad x \in \Omega, \tag{3.4.3}$$

which admits three types of stationary solutions. We can write each stationary solution $u(x)$ in the form

$$u = 1\chi_A + (-1)\chi_B + 0\chi_{\Omega\setminus(A\cup B)}, \tag{3.4.4}$$

where A, B are any measurable subsets of Ω. If all the three sets in (3.4.4) have non-zero measure, we say that u is a *three-phase* solution; if exactly one of them has zero measure, we say that u is a *two-phase* solution; otherwise u is one of the three *one-phase* solutions, ± 1 or 0.

In what follows we shall be particularly interested in two-phase solutions to (3.4.3) on domains of size $|\Omega| = 1$ and their continuations to solutions to (3.4.1) with γ small enough. For a fixed number $s \in (0, 1)$ and $a, b \in \{-1, 0, 1\}$, we denote by $[\![a, b]\!]$, the set of stationary solutions u that take the value a on a set of measure s, and b on a set of measure $1 - s$. Obviously, $[\![1, 0]\!]$ and $[\![0, 1]\!]$ are the same sets if $s = 1/2$, but different otherwise.

The results of this section hold for any $\varepsilon > 0$, and its value is not important in the calculations. Hence we shall fix $\varepsilon = 1$, which implies $J_\varepsilon(\cdot) = J(\cdot)$. Let us denote by $G(u, \gamma)$ the function in the left-hand side of equation (3.4.1).

Theorem 3.13 *Let $s \in (0, 1)$ and let $\hat{u}$ be an $[\![a, b]\!]$ solution of (3.4.3). There exists $\gamma^* > 0$ such that every such solution has a locally unique continuation for all $0 < \gamma < \gamma^*$.*

Proof. We prove this theorem by applying the Implicit Function Theorem. Let us define the following sets:

$$\Omega_+(\hat{u}) = \{x \in \Omega; \quad \hat{u}(x) = +1\},$$

$$\Omega_0(\hat{u}) = \{x \in \Omega; \quad \hat{u}(x) = 0\},$$

$$\Omega_-(\hat{u}) = \{x \in \Omega; \quad \hat{u}(x) = -1\}.$$

The stationary state $\hat{u} = [\![a, b]\!]$ satisfies $G(\hat{u}, 0) = 0$. We prove now that in $L^\infty(\Omega)$ every solution $\hat{u}$ of $G(u, 0) = 0$ is isolated, and hence locally unique. Let us suppose that there exists a sequence $\{h_n\}_n$ such that $\|h_n\|_\infty \to 0$ and $f(\hat{u} + h_n) = 0$ for all n. For small enough h, we have that

$$f(\hat{u} + h) = f(\hat{u}) + f'(\hat{u})h + \omega(\hat{u}, h), \quad \text{where } \lim_{\|h\|_\infty \to 0} \frac{\|\omega(\hat{u}, h)\|_\infty}{\|h\|_\infty} = 0. \quad (3.4.5)$$

By writing (3.4.5) for h_n and using the fact that $f(\hat{u}) = 0$, we get

$$-f'(\hat{u})h_n = \omega(\hat{u}, h_n), \quad \text{for all } n,$$

which implies that $\lim_{\|h_n\|_\infty \to 0} \|f'(\hat{u})\|_\infty = 0$. This is not true, since $f(u) = u^3 - u$, and so $-f'(\hat{u}) \in \{1, -2\}$. Thus, each solution $\hat{u}$ of $G(u, 0) = 0$ is isolated in $L^\infty(\Omega)$. The zero $(\hat{u}, 0)$ of G has a locally unique continuation around $\gamma = 0$ if, by the Implicit Function Theorem, the map G is continuously differentiable, the derivative of G with respect to u, denoted by DG, is invertible at $(\hat{u}, 0)$ and $DG^{-1}(\hat{u}, 0)$ is bounded. We want now to find $DG(\hat{u}, 0)$. For all $v \in L^\infty(\Omega)$ we have

$$\begin{aligned}\frac{d}{dh}G(u + hv, \gamma)|_{h=0} = \frac{d}{dh}\{\gamma \int_\Omega J_\varepsilon(|x - y|)((u + hv)(y) - (u + hv)(x))dy - \\ -f((u + hv)(x))\}|_{h=0} \\ = \gamma \int_\Omega J_\varepsilon(|x - y|)(v(y) - v(x))dy - f'(u)v,\end{aligned}$$

whence

$$DG(\hat{u}, 0) = -f'(\hat{u}).$$

Since $-f'(\hat{u}) \in \{1, -2\}$, $DG(\hat{u}, 0)$ is invertible, with the inverse $DG^{-1}(\hat{u}, 0)$ being the operator of multiplication by the L^∞ function

$$g(x) = \chi_{\Omega_0(\hat{u})}(x) - \frac{1}{2}\chi_{\Omega_-(\hat{u}) \cup \Omega_+(\hat{u})}(x).$$

Hence $\|DG^{-1}(\hat{u}, 0)\| \leq 1$ for all $s \in (0, 1)$ and by the Implicit Function Theorem there is $\gamma^* > 0$ such that $G(u, \gamma) = 0$ has a locally unique solution $u(\gamma)$, $u(0) = u_0$ for all s in $(0, 1)$, for all $0 < \gamma < \gamma^*$. □

Remark 3.14 Following the remark of MacKay & Sepulchre [73], one can find a common lower bound γ^*, for which all stationary states $[\![a, b]\!]$ have a locally

unique continuation to solutions of (3.4.1) with $0 < \gamma < \gamma^*$. We also note that the upper bounds are clearly dependent on s, as we shall see in Section 3.5 for the particular case $J(\cdot) \equiv 1$. Obviously, the above result holds for all $|\gamma| < \gamma^*$, but in our context the parameter γ has to be positive.

Since $G(u, \gamma)$ depends analytically on γ, regular perturbation expansions in γ for solutions of (3.4.1) converge for γ sufficiently small. The next lemma states that if γ is sufficiently small, then the locally unique continuations of a solution $\hat{u} = [\![1, 0]\!]$ will change sign in Ω; it will be slightly less than 1 on the subset of Ω where $\hat{u} = 1$, and slightly less than 0 on the subset of Ω where $\hat{u} = 0$. This information is useful in the next subsection when we prove the non-coarsening property of solutions of (3.3.1).

Lemma 3.15 *If $u(0) = \hat{u}$ is any $[\![1, 0]\!]$ solution, then for sufficiently small $\gamma > 0$, the solution $u(\gamma)$ of (3.4.1) satisfies $u(\gamma)(x) = -\gamma C_1(x) + \mathcal{O}(\gamma^2)$ on $\Omega_0(\hat{u})$ and $u(\gamma)(x) = 1 - \gamma C_2(x) + \mathcal{O}(\gamma^2)$ on $\Omega_+(\hat{u})$, where $C_1(x)$, $C_2(x)$ are both $\mathcal{O}(1)$ in Ω and positive.*

Proof. We seek a solution of (3.4.1) in the form

$$u(\gamma)(x) = \hat{u}(x) + \gamma u_1(x) + \mathcal{O}(\gamma^2). \tag{3.4.6}$$

Powers of γ^0 give

$$\hat{u}(x) - \hat{u}^3(x) = 0, \quad x \in \Omega,$$

which has solution

$$\hat{u}(x) = \begin{cases} 0, & x \in \Omega_0(\hat{u}) \\ \\ 1, & x \in \Omega_+(\hat{u}). \end{cases} \tag{3.4.7}$$

Powers of γ give

$$\int_\Omega J(|x - y|)(\hat{u}(y) - \hat{u}(x))dy + u_1(x) - 3\hat{u}^2(x)u_1(x) = 0, \quad x \in \Omega,$$

from which we can get $u_1(x)$. If we denote by

$$K(x) = \int_\Omega J(|x - y|)dy,$$

then $0 \leq K(x) \leq 1$ and we have

$$u_1(x) = \frac{\int_\Omega J(|x-y|)(\hat{u}(y)-\hat{u}(x))\,dy}{3\hat{u}^2(x)-1} \tag{3.4.8}$$

$$= \frac{\int_{\Omega_+(\hat{u})} J(|x-y|)dy - K(x)\hat{u}(x)}{3\hat{u}^2(x)-1}$$

$$= \begin{cases} -\int_{\Omega_+(\hat{u})} J(|x-y|)dy, & x \in \Omega_0(\hat{u}) \\ \\ -\frac{1}{2}\int_{\Omega_0(\hat{u})} J(|x-y|)dy, & x \in \Omega_+(\hat{u}). \end{cases}$$

$$= \begin{cases} -C_1(x), & x \in \Omega_0(\hat{u}) \\ -C_2(x), & x \in \Omega_+(\hat{u}), \end{cases} \tag{3.4.9}$$

where C_1 and C_2 are positive functions of x since J is a non-negative kernel, and $C_1(x)$, $C_2(x)$ are $\mathcal{O}(1)$ in Ω (being bounded in Ω, as a consequence of $J \in L^1(\mathbb{R})$). The conclusion of the lemma follows by substituting the expressions of $\hat{u}(x)$ and $u_1(x)$ into (3.4.6). □

Remark 3.16 Obviously, a similar statement can be made for continuations of $[\![-1, 0]\!]$ solutions. We can prove that if $u(0) = \hat{u}$ is any $[\![-1, 0]\!]$ solution, then for sufficiently small $\gamma > 0$, the solution $u(\gamma)$ of (3.4.1) satisfies

$$u(\gamma)(x) = \gamma C_3(x) + \mathcal{O}(\gamma^2) \quad \text{on} \quad \Omega_0(\hat{u}),$$

and

$$u(\gamma)(x) = -1 + \gamma C_4(x) + \mathcal{O}(\gamma^2) \quad \text{on} \quad \Omega_+(\hat{u}),$$

where $C_3(x)$, $C_4(x)$ are both $\mathcal{O}(1)$ in Ω and positive.

As we have noted in Section 2.2.2, the Allen-Cahn equation possesses a compact attractor. The next theorem shows that this is not the case for (3.3.1).

Theorem 3.17 *For sufficiently small γ the set of equilibria is not compact, so the dynamical system generated by (3.3.1) cannot have a compact attractor.*

Proof. We shall construct a sequence of equilibria which does not contain any convergent subsequence. Let us take a sequence $\{\hat{u}_n\}$, $n = 1, 2, \ldots$, of two-phase solutions of the equation (3.4.3), each element of the sequence being of one of the types $[\![-1, 0]\!]$, $[\![0, -1]\!]$, $[\![1, 0]\!]$, or $[\![0, 1]\!]$, where two elements of the same type differ by a set of positive measure, such that

$$\|\hat{u}_i - \hat{u}_j\|_\infty = 1, \quad \text{for all } i \neq j, \quad i, j = 1, 2, \ldots.$$

By Theorem 3.13, for small enough γ each $\hat{u}_n$ has a locally unique continuation, which we denote by $u_n(\gamma)$. Using the representation (3.4.6) of $u(\gamma)(x)$, where u_1 is given by (3.4.8), we have:

$$\begin{aligned} u_n(\gamma)(x) &= \hat{u}_n(x) + \gamma u_{n1}(x) + \omega_n(x) \\ &= \hat{u}_n(x) - \gamma \left(\frac{\int_\Omega J(|x-y|)(\hat{u}_n(y) - \hat{u}_n(x))dy}{1 - 3\hat{u}_n^2(x)} \right) + \omega_n(x), \end{aligned}$$

where $\omega_n(x)$ is of order $\mathcal{O}(\gamma^2)$. Using the fact that the operator A_1 is bounded in $L^\infty(\Omega)$ and the triangle inequality, we have that for any two elements of the sequence, $u_i(\gamma)$ and $u_j(\gamma)$,

$$\begin{aligned} \|u_i(\gamma) - u_j(\gamma)\|_\infty &\geq \|\hat{u}_i - \hat{u}_j + \gamma u_{i1} - \gamma u_{j1}\|_\infty - \|\omega_i - \omega_j\|_\infty \\ &\geq \|\hat{u}_i - \hat{u}_j + \gamma u_{i1} - \gamma u_{j1}\|_\infty + \mathcal{O}(\gamma^2) \\ &\geq 1 - \gamma \|u_{i1} - u_{j1}\|_\infty + \mathcal{O}(\gamma^2) \\ &\geq 1 - \gamma(\|u_{i1}\|_\infty + \|u_{j1}\|_\infty) + \mathcal{O}(\gamma^2) \\ &\geq 1 - \gamma \left(\frac{2\|\hat{u}_i\|_\infty}{\|3\hat{u}_i^2 - 1\|_\infty} + \frac{2\|\hat{u}_j\|_\infty}{\|3\hat{u}_j^2 - 1\|_\infty} \right) + \mathcal{O}(\gamma^2) \\ &\geq 1 - \gamma C + \mathcal{O}(\gamma^2), \end{aligned}$$

for some positive constant C. The last inequality implies that for sufficiently small γ the sequence $\{u_n(\gamma)\}_n$ is not Cauchy, and thus $\{u_n(\gamma)\}_n$ is not convergent. In fact, this sequence of equilibrium points does not contain any convergent subsequence. This means that the set of equilibria cannot be compact, which ends the proof of the theorem. □

Remark 3.18 The lack of compactness of equilibria prevents the semigroup $\{T(t),\, t \geq 0\}$ from being a gradient system, and thus we cannot apply the the-

ory of Hale [62] for such systems, in particular we cannot apply Theorem 2.10, Section 2.1.

3.5 Bifurcation diagram and coarsening

We shall consider firstly the particular case $J(\cdot) \equiv 1$ and $\varepsilon = 1$, in which case we draw and discuss the bifurcation diagram for two-phase solutions, then we define what we mean by 'coarsening' and examine the coarsening of solutions of (3.3.1). At the end of the section we give general results for coarsening of solutions to (3.3.1) in the case $J(\cdot) \geq 0$. We set $|\Omega| = 1$.

Let us take $J(\cdot) \equiv 1$. The equation (3.3.1) becomes

$$u_t = \gamma \left(\int_\Omega u(y)dy - u \right) + u - u^3, \quad x \in \Omega,\ t > 0, \tag{3.5.1}$$

and the steady states are solutions of the equation

$$0 = \gamma \left(\int_\Omega u(y)dy - u \right) + u - u^3, \ x \in \Omega. \tag{3.5.2}$$

The spectrum of the linearization around a stationary solution $v(x)$ is easily computed. Linearizing, we get

$$u_t = \gamma \left(\int_\Omega u(y)dy - u \right) + (1 - 3v^2)u, \quad x \in \Omega,\ t > 0.$$

If we look for solutions of the form $u(x,\, t) = e^{\lambda t}\phi(x)$, we obtain the eigenvalue problem

$$(\lambda + \gamma + 3v^2(x) - 1)\,\phi(x) = \gamma \int_\Omega \phi(y)\,dy. \tag{3.5.3}$$

Multiplying both sides by ϕ and then integrating, we have

$$\int_\Omega (\lambda + \gamma + 3v^2(x) - 1)\,\phi^2(x)\,dx = \gamma \left(\int_\Omega \phi(x)\,dx \right)^2, \tag{3.5.4}$$

which combined with the following inequality

$$\left(\int_\Omega \phi(x)\,dx \right)^2 \leq \int_\Omega \phi^2(x)\,dx,$$

gives

$$\int_\Omega (\lambda + 3v^2(x) - 1)\,\phi^2(x)\,dx \leq 0. \tag{3.5.5}$$

If $v(x)$ is such that $3v^2(x) - 1 > 0$ for all $x \in \Omega$, then the last inequality implies that all the eigenvalues are negative. In particular, we get that the one-phase steady states $v \equiv \pm 1$ are linearly stable. For $v \equiv 0$ and $\gamma = 1$ in (3.5.3) we get a zero eigenvalue for which any function ϕ of zero mass is an eigenfunction.

One can also draw the global bifurcation diagram for two-phase and three-phase solutions, but here we shall treat only the case of two-phase solutions. Clearly, all multi-phase solutions in this case are piecewise constant. Any two-phase solution of (3.5.2) has the form

$$u(x) = u_1\chi_A + u_2\chi_{\Omega\setminus A},$$

where $A \subset \Omega$ and $u_1 \neq u_2$. Setting $|A| = s$, $s \in (0, 1)$, we obtain the following system of equations for u_1, u_2:

$$\begin{cases} \gamma[su_1 + (1-s)u_2 - u_1] + u_1 - u_1^3 = 0 \\ \gamma[su_1 + (1-s)u_2 - u_2] + u_2 - u_2^2 = 0. \end{cases} \tag{3.5.6}$$

We analyse this system using MAPLE. Subtracting the two equations and eliminating the non-zero term $u_1 - u_2$, we get

$$u_1^2 + u_1u_2 + u_2^2 + \gamma - 1 = 0. \tag{3.5.7}$$

We observe that the system (3.5.6) has solutions only for $\gamma < 1$; if $\gamma \geq 1$, the equation (3.5.2) has only one-phase solutions. Eliminating u_1 in (3.5.6) by taking the resultant, we have a single equation in u_2, that is:

$$u_2^6 + (3\gamma s - 2)u_2^4 + (3\gamma^2 s^2 - 3\gamma s + 1)u_2^2 + \gamma^3 s^2 - \gamma^2 s^2 = 0. \tag{3.5.8}$$

We fix s and treat γ as a bifurcation parameter. We obtain the bifurcation diagrams shown in Figures 3.1 and 3.2, also obtained in [32]. As we can see in Figure 3.2, the second pitchfork bifurcation is broken if $s \neq 1/2$. Here we have represented the stable solutions by solid lines and the unstable ones by broken lines. We can draw the following conclusion: if $\gamma < 1$, then the equation (3.4.1) admits an uncountable number of non-constant solutions, since each branch represented in these figures corresponds to an uncountable equivalence class of stationary solutions. We can also prove the following Proposition:

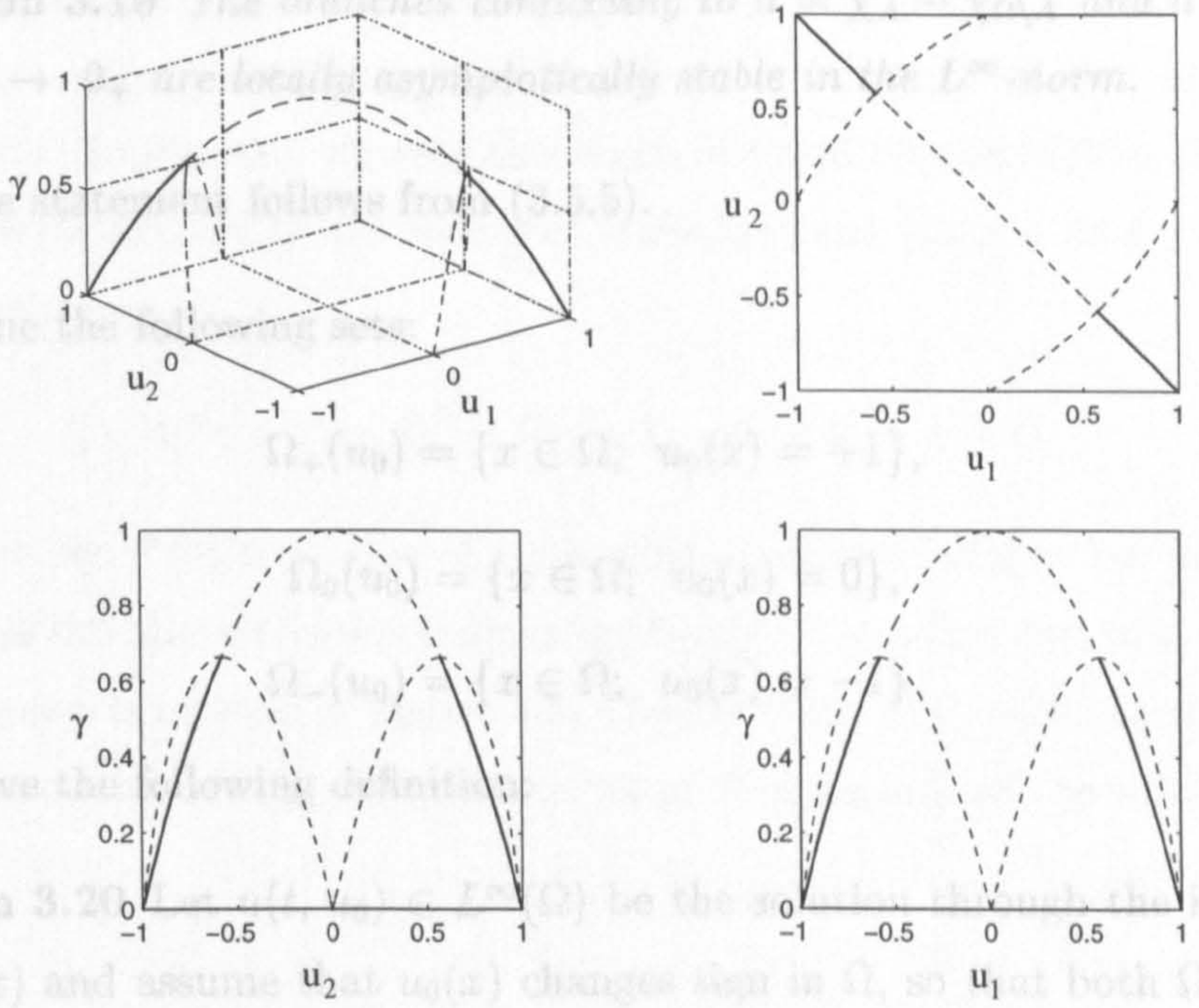

Figure 3.1: Solutions of (3.5.6) in the case $s = 0.5$.

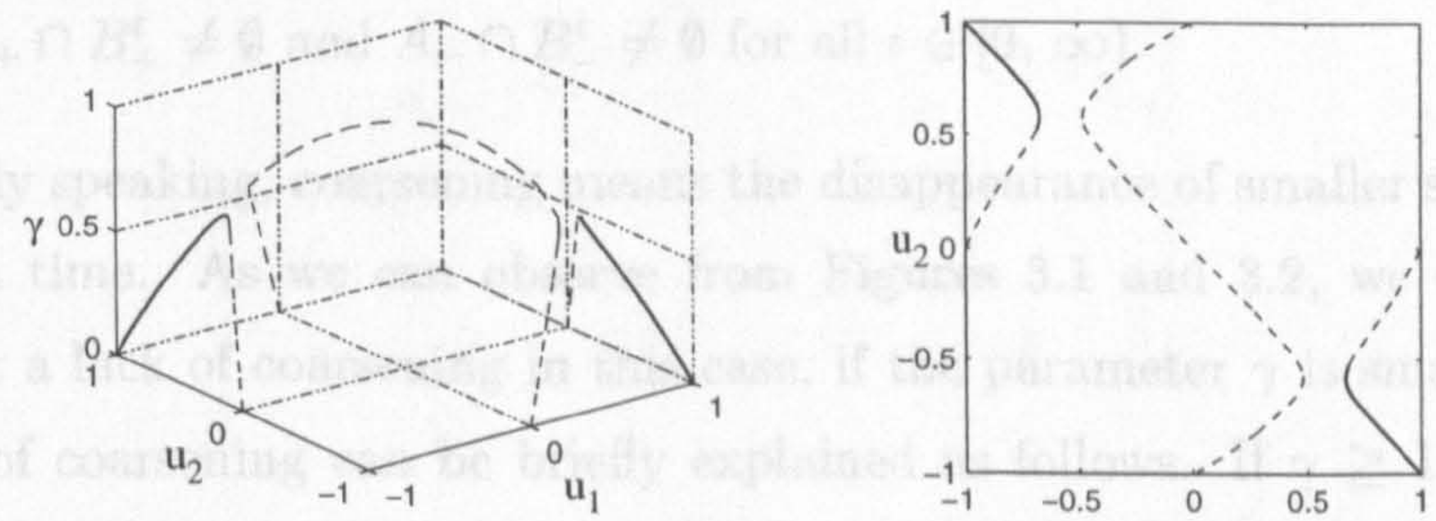

Figure 3.2: Solutions of (3.5.6) in the case $s = 0.51$.

Proposition 3.19 *The branches connecting to* $u = \chi_A - \chi_{\Omega\setminus A}$ *and* $u = -\chi_A + \chi_{\Omega\setminus A}$ *as* $\gamma \to 0_+$ *are locally asymptotically stable in the* L^∞*-norm.*

Proof. The statement follows from (3.5.5). □

Let us define the following sets:

$$\Omega_+(u_0) = \{x \in \Omega;\ \ u_0(x) = +1\},$$

$$\Omega_0(u_0) = \{x \in \Omega;\ \ u_0(x) = 0\},$$

$$\Omega_-(u_0) = \{x \in \Omega;\ \ u_0(x) = -1\}.$$

We now give the following definition:

Definition 3.20 Let $u(t, u_0) \in L^\infty(\Omega)$ be the solution through the initial condition $u_0(x)$ and assume that $u_0(x)$ changes sign in Ω, so that both $\Omega_+(u_0)$ and $\Omega_-(u_0)$ have nonzero measure. We say that the solution u *does not coarsen* if for each component A_+ of the set $\Omega_+(u_0)$ and component A_- of $\Omega_-(u_0)$ there exist non-empty sets B_+^t and B_-^t such that $u(t, u_0)$ is positive on B_+^t and negative on B_-^t and $A_+ \cap B_+^t \neq \emptyset$ and $A_- \cap B_-^t \neq \emptyset$ for all $t \in [0, \infty)$.

Roughly speaking, coarsening means the disappearance of smaller scale structures with time. As we can observe from Figures 3.1 and 3.2, we can rather talk about a lack of coarsening in this case, if the parameter γ is small enough. The lack of coarsening can be briefly explained as follows. If $\gamma \geq 1$, then any initial condition lies in the domain of attraction of a stable constant solution, either $u \equiv -1$ or $u \equiv +1$. As γ is decreased below 1, the equation (3.3.1) has an uncountable number of non-constant steady state solutions. As we shall prove rigorously in Theorem 3.22, if the initial condition u_0 changes sign in Ω and γ is small enough, then the solution of (3.3.1) starting from u_0, $u(t; u_0)$, will preserve the number of changes of sign and consequently, the stationary solution will have the same property. Thus, this initial data will be attracted by a non-constant equilibrium which has the the same pattern of change of sign as u_0, which means that the solution u cannot coarsen at all.

We would like now to find the values of γ at which a second bifurcation phenomenon occurs and, in particular, if the occurrence of this phenomenon depends on s. To this end, we need the values of γ and s for which the discriminant of (3.5.8) with respect to u_2 vanishes. This happens when s and γ satisfy the following relation:

$$27\gamma^4 s^2(1-s)^2 - 18\gamma^2 s(1-s) + 4\gamma - 1 = 0.$$

If we denote by $\gamma^*(s)$ the value of γ for which a second bifurcation phenomenon occurs, then the above relation defines implicitly γ^* as a function of s. The graph of this function is plotted in Figure 3.3. Clearly $\gamma^*(s) \not\to 0$, which means that the second bifurcation occurs at a positive value of γ, regardless the value of s.

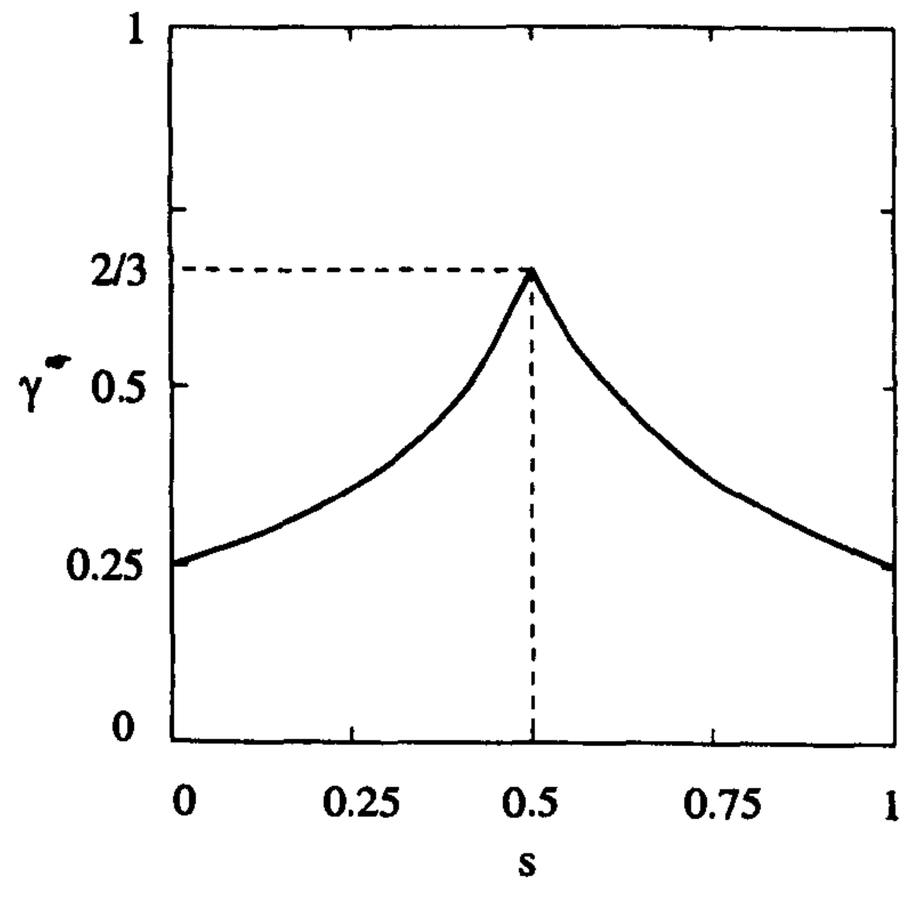

Figure 3.3: The relationship between γ^* and s.

We now remove the restrictions $J(\cdot) \equiv 1$ and $\varepsilon = 1$. Let us fix $\gamma = 1$, and consider $f(u) = u^3 - u$ and the kernel J such that

$$J \in C^2(\mathbb{R}), \quad J(-x) = J(x), \quad J(\cdot) \geq 0, \quad \int_{\mathbb{R}} J(x)\,dx = 1, \text{ and}$$

$$\int_{\mathbb{R}} J(x)x^2\,dx < \infty.$$

The following result is concerned with coarsening of solutions to (3.3.1), and is due to Fife and Wang [48].

Theorem 3.21 *Assume that the kernel J satisfies the above conditions, and suppose that the initial data u_0 has $\|u_0\|_{C^2(\mathbb{R})}$ finite. Then there exist three positive constants, τ_0 (depending on f) and M_0, M_1 (both depending on f and $\|u_0\|_{C^2}$), such that for sufficiently small $\varepsilon > 0$ we have*

(*i*) *if x is such that $u_0(x) \geq M_0\sqrt{\varepsilon}\,|\ln\varepsilon|$, then $u(x,\,t) \geq 1 - M_1\varepsilon$, for all $t \geq \tau_0\varepsilon|\ln\varepsilon|$, and*

(*ii*) *if x is such that $u_0(x) \leq -M_0\sqrt{\varepsilon}\,|\ln\varepsilon|$, then $u(x,\,t) \leq -1 + M_1\varepsilon$, for all $t \geq \tau_0\varepsilon|\ln\varepsilon|$.*

Proof. See [48], Theorem 1. □

The theorem shows that if the initial data changes sign and ε is small enough, the space is partitioned into state regions divided by thin layers which are generated in a time scale $\mathcal{O}(\varepsilon|\ln\varepsilon|)$. In other words, a solution which starts from an initial data u_0 that changes sign does not coarsen in time if the value of ε is small enough. We can prove a similar result for small enough values of the parameter $\gamma > 0$. Our theorem considers a more general class of initial data which includes discontinuous functions, and the assumptions on J are less restrictive.
We fix $\varepsilon = 1$, while γ is a positive real number.

Theorem 3.22 *For every kernel J satisfying $(\mathcal{H}_1)$, and every initial condition $u_0 \in L^\infty(\Omega)$ that changes sign, $\|u_0\|_\infty < 1$, there is a value $\gamma_0 = \gamma_0(u_0) > 0$, such that for all $0 < \gamma < \gamma_0$ the solution through u_0 does not coarsen at all.*

The idea of the proof is simple: we aim to trap the initial data u_0 between a pair of two-phase stationary solutions of (3.3.1) and thus, by the comparison principle stated in Lemma 3.5, the solution $u(t,\,u_0)$ will remain trapped at each time t. Consequently, the solution u cannot coarsen at all.

The sets $\Omega_+(u_0)$ and $\Omega_-(u_0)$ may have up to an infinite components. Let us denote by A_+^i the i-th component of $\Omega_+(u_0)$, and by A_j^- the j-th component of $\Omega_-(u_0)$. Before starting the proof we give the following definition:

Definition 3.23 We say that a pair $(u_-,\,u_+)$ is a *blocking pair for u_0* if

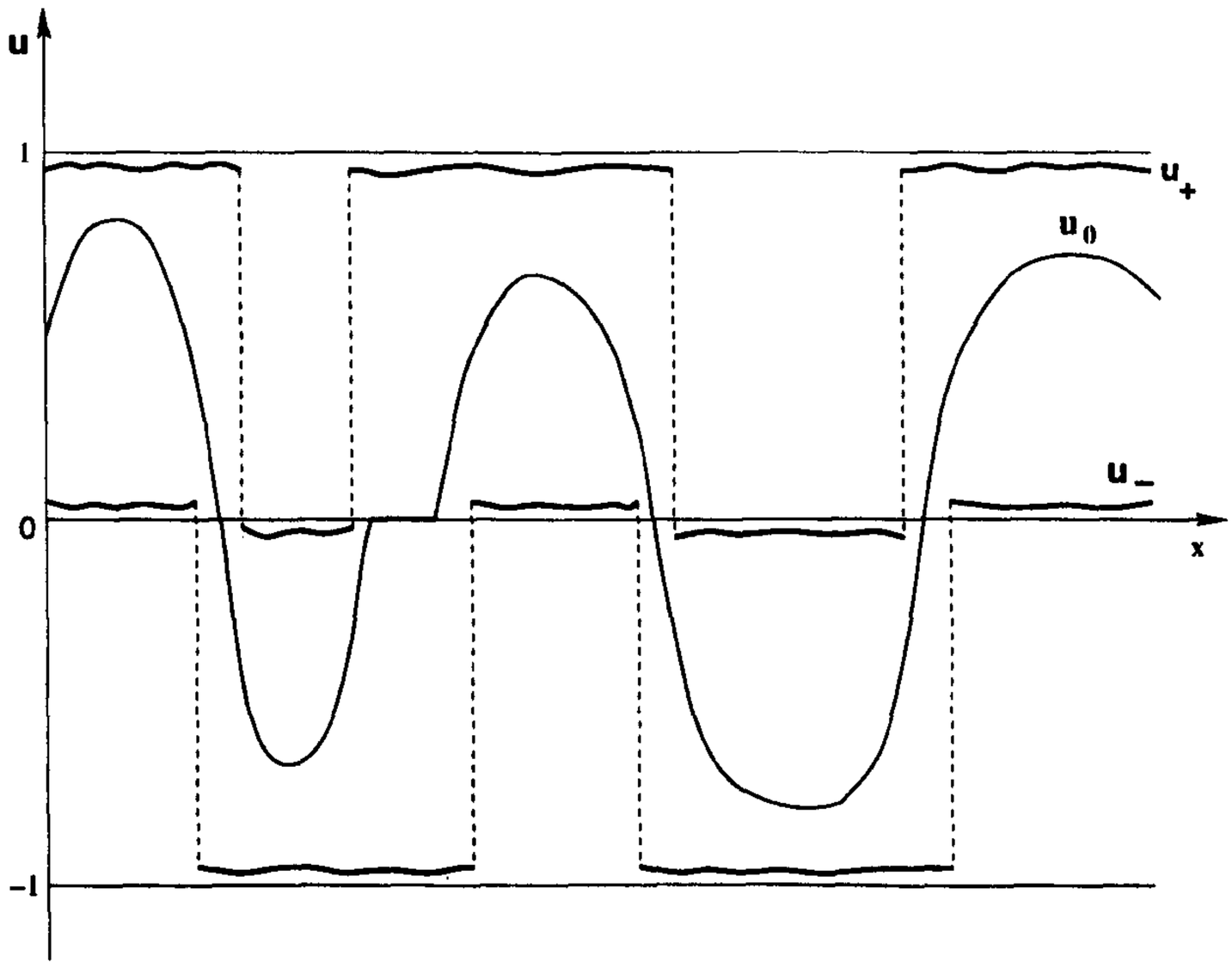

Figure 3.4: A blocking pair for u_0.

1. $u_- \leq u_0 \leq u_+$, and

2. for each i, j, the function u_+ is positive on a set that contains A_+^i and negative on a subset of A_j^-; and similarly, the function u_- is positive on a subset of A_+^i and negative on set containing A_j^-.

Proof. (*of Theorem 3.22*) It remains only to show that for γ sufficiently small every initial data satisfying the conditions in the theorem admits a blocking pair. For a given $u_0 \in L^\infty(\Omega)$ that changes sign, we can find a pair of two-phase solutions of (3.4.3), say $\underline{u}(x)$ and $\overline{u}(x)$, such that

1. $\underline{u}$ is either of type $[\![-1, 0]\!]$ or $[\![0, -1]\!]$;

2. $\overline{u}$ is either of type $[\![1, 0]\!]$ or $[\![0, 1]\!]$;

3. $\underline{u}(x) \leq u_0(x) \leq \overline{u}(x)$, for all $x \in \Omega$.

By Theorem 3.13 we can find a lower bound $\gamma^* > 0$ such that each of $\underline{u}(x)$ and $\overline{u}(x)$ have a unique continuation for all $0 < \gamma < \gamma^*$. Let us denote these continuations by $u_-(\gamma)(x)$ and $u_+(\gamma)(x)$, respectively. Using the properties of

these two stationary solutions (see Lemma 3.15), we can choose a small enough γ, say $\overline{\gamma}$, such that $u_\pm \equiv u_\pm(\overline{\gamma})$ satisfies

$$u_-(x) \leq u_0(x) \leq u_+(x), \text{ for all } x \in \Omega.$$

We claim that (u_-, u_+) is a blocking pair for u_0, and thus the theorem is proved. See Figure 3.4 for an illustration of the construction. □

Remark 3.24 Clearly, the comparison principle implies that a solution $u(t, u_0)$ starting from a non-negative (resp. non-positive) initial data u_0 will also be non-negative (resp. non-positive). Theorem 3.22 states that for small enough γ the evolution system does not define a length-scale.

Remark 3.25 Let us mention that this theorem may also be adapted for a convex bounded domain $\Omega \subset \mathbb{R}^n$ (see also [32]).

In the remainder of this section, we shall state and prove a generalization of Theorem 3.22, which does not contain any reference to a kernel J. Let us consider the following problem on $L^\infty(\Omega)$:

$$\begin{cases} u_t = A_\sigma u - f(u) \\ u(0) = u_0, \end{cases} \tag{3.5.9}$$

with the following hypotheses on A_σ:

$$\begin{cases} A_\sigma \text{ is bounded, linear operator on } L^\infty(\Omega) \\ A_\sigma u_{min} \geq 0, \quad A_\sigma u_{max} \leq 0 \\ A_\sigma u = 0 \quad \text{implies } u \equiv const. \\ A_\sigma u = \mathcal{O}(\sigma^2) \text{ as } \sigma \to 0. \end{cases} \tag{3.5.10}$$

The following arguments may be adapted for any bistable function (as in $(\mathcal{H}_2)$) and, for simplicity, we take here $f(u) = u^3 - u$.

The global existence and uniqueness of a solution $u(x, t; u_0) \in C^1([0, \infty); L^\infty(\Omega))$ follows exactly as in Section 3.3. Since A_σ is a bounded operator on $L^\infty(\Omega)$, for all $\sigma > 0$, we may as well construct a unique local solution for backward time. We shall prove first that if A_σ satisfies $(3.5.10)_1 - (3.5.10)_3$, then the comparison principle for solutions of (3.5.9) holds. We start with a lemma:

Lemma 3.26 *Let A_σ be an operator satisfying $(3.5.10)_1$ – $(3.5.10)_3$, and let $c(x, t)$ be a bounded function in $\bar{\Omega} \times [0, T]$. If $w(x, t)$ is a solution of*

$$w_t = A_\sigma w - c(x, t)w, \tag{3.5.11}$$

such that $w(x, 0) > 0$ on Ω, then

$$w(x, t) > 0 \quad in\ \Omega \times (0, T).$$

Proof. Suppose, by contradiction, that there exists a first time $t_0 \in (0, T]$ such that $w(x_0, t_0) = 0$ for some $x_0 \in \bar{\Omega}$. It follows that

$$\frac{\partial}{\partial t} w(x_0, t_0) \leq 0,$$

and from (3.5.11) we obtain

$$A_\sigma w(x_0, t_0) \leq 0. \tag{3.5.12}$$

Since $w(x, t_0) \geq w(x_0, t_0) = 0$ for all $x \in \bar{\Omega}$, the hypothesis $(3.5.10)_2$ implies

$$A_\sigma w(x_0, t_0) \geq 0.$$

This relation combined with (3.5.12) yield

$$A_\sigma w(x_0, t_0) = 0,$$

and thus $w(x, t_0) = const.\ (= 0)$ for all $x \in \bar{\Omega}$, by $(3.5.10)_3$. By backward uniqueness of the initial value problem (3.5.11) + $\{w(x, t_0) = 0\}$, we get $w \equiv 0$. The contradiction arises from the fact that t_0 was chosen to be the first time for which $w(x, t_0) = 0$. □

Proposition 3.27 Let u and v be solutions of $(3.5.9)_1$ in $\Omega \times [0, T]$ satisfying

$$u(x, 0) < v(x, 0), \qquad x \in \Omega.$$

Then we have

$$u(x, t) < v(x, t), \quad \text{for all } (x, t) \in \Omega \times (0, T).$$

Proof. Let $w = v - u$. Then

$$w_t = A_\sigma w - c(x, t)w, \tag{3.5.13}$$

where

$$c(x, t) = \frac{f(v) - f(u)}{v - u}$$

is a bounded function, since $f \in C^1$. It follows from the previous lemma that $w(x, t) > 0$ for all $(x, t) \in \Omega \times (0, T)$, which ends the proof. □

We can now prove the following theorem:

Theorem 3.28 *Let A_σ be such that the conditions (3.5.10) are satisfied. For every initial condition $u_0 \in L^\infty(\Omega)$ that changes sign, $\|u_0\|_\infty < 1$, there is a value $\sigma_0 = \sigma_0(u_0) > 0$, such that for all $0 < \sigma < \sigma_0$ the solution of (3.5.9) through u_0 does not coarsen at all.*

Proof. The proof follows exactly the steps of the proof of Theorem 3.22. Due to the boundedness of A_σ, one can apply the Implicit Function Theorem to obtain locally unique continuations of solutions of (3.4.3) to solutions of $A_\sigma u = f(u)$ with σ small enough. Thus, one can find a lower bound σ^* so that each of $\underline{u}(x)$ and $\overline{u}(x)$ (defined as in the proof of Theorem 3.22) have a unique continuation for all $0 < \sigma < \sigma^*$. Let us denote these continuations by $u_-(\sigma)(x)$ and $u_+(\sigma)(x)$. It remains to show the existence of a blocking pair for $u_0(x)$, which completes the proof of the theorem. To this end, one needs to prove that these continuations have similar properties to $u_-(\gamma)(x)$ and $u_+(\gamma)(x)$ (see Lemma 3.15). We shall prove a variant of Lemma 3.15, which is Lemma 3.29, concerning properties of continuations of $[\![1, 0]\!]$ solutions. A similar result can be proved for continuations of $[\![-1, 0]\!]$ solutions. □

Lemma 3.29 *Let A_σ be an operator that satisfies (3.5.10), and $u(0) = \hat{u}$ any $[\![1, 0]\!]$ solution of $f(u) = 0$. Then, for sufficiently small $\sigma > 0$, the solution $u(\sigma)$ of $A_\sigma u = f(u)$ satisfies $u(\sigma)(x) = -C_1(x)\sigma^2 + \mathcal{O}(\sigma^3)$ on $\Omega_0(\hat{u})$ and $u(\sigma)(x) = 1 - C_2(x)\sigma^2 + \mathcal{O}(\sigma^3)$ on $\Omega_+(\hat{u})$, where $C_1(x)$, $C_2(x)$ are both $\mathcal{O}(1)$ in Ω and positive.*

Proof. We seek a solution of $A_\sigma u = f(u)$ in the form:

$$u(\sigma)(x) = \hat{u}(x) + \sigma u_1(x) + \sigma^2 u_2(x) + \mathcal{O}(\sigma^3). \tag{3.5.14}$$

We obtain:

$$A_\sigma \hat{u} + \mathcal{O}(\sigma^3) = (\hat{u} + \sigma u_1 + \sigma^2 u_2)^3 - \hat{u} - \sigma u_1 - \sigma^2 u_2 + \mathcal{O}(\sigma^3). \tag{3.5.15}$$

Equating the corresponding $\mathcal{O}(1)$ terms, we get

$$\hat{u} - \hat{u}^3 = 0, \;\; x \in \Omega,$$

which has solution

$$\hat{u}(x) = \begin{cases} 0, & x \in \Omega_0(\hat{u}) \\ \\ 1, & x \in \Omega_+(\hat{u}). \end{cases} \tag{3.5.16}$$

Powers of σ give

$$(3\hat{u}^2 - 1)u_1 = 0,$$

from which we get $u_1 \equiv 0$. From (3.5.15) we also get

$$A_\sigma \hat{u} = (3\hat{u}^2 - 1)u_2\sigma^2 + \mathcal{O}(\sigma^3). \tag{3.5.17}$$

Due to $(3.5.10)_2$ and $(3.5.10)_4$, the previous relation implies that

$$u_2(x) = \begin{cases} -C_1(x), \text{ on } \Omega_0(\hat{u}) \\ \\ -C_2(x), \text{ on } \Omega_+(\hat{u}), \end{cases}$$

which completes the proof. □

Remark 3.30 As we shall see, by considering particular forms of A_σ, one can get from this theorem the results of Theorems 3.22 and 3.21 (in the latter case some additional assumptions are required). In Section 2.2.2, we have seen that solutions of (2.2.14) do coarsen to a constant solution, regardless the choice of ϵ or initial data u_0. The differences between the coarsening properties of (2.2.14) and (3.3.1) are mainly due to the fact that A_ϵ is bounded, and the operator $\epsilon^2 \Delta u$ is unbounded. Thus $\epsilon^2 \Delta u$ fails to obey the first requirement in (3.5.10), which makes Theorem 3.28 inapplicable for solutions of (2.2.14).

(1) Let us consider a kernel J satisfying $(\mathcal{H}_1)$. One can easily check that the operator

$$A_\sigma u(x) = \sigma^2 \int_\Omega J(|x-y|)(u(y)-u(x))\,dy,$$

satisfies the hypotheses (3.5.10) (see also Lemma 3.2). In fact, this is the operator γA_ε (see (3.3.3)) with $\gamma = \sigma^2$ and $\epsilon = 1$. Thus, the previous theorem proves the non-coarsening of solutions of (3.3.1) for small enough values of γ, i.e. the result of Theorem 3.22.

(2) We now consider the operator

$$A_\sigma u(x) = \frac{1}{\sigma}\int_{\mathbb{R}} J(\frac{|x-y|}{\sigma})(u(y)-u(x))\,dy, \tag{3.5.18}$$

and, in addition to $(\mathcal{H}_1)$, assume that

$$\rho_2 := \int_{\mathbb{R}} J(|x|)x^2\,dx < \infty. \tag{3.5.19}$$

Obviously, the operator (3.5.18) is bounded and linear on $L^\infty(\Omega)$, and satisfies the hypotheses $(3.5.10)_2$ and $(3.5.10)_3$. We would like to see whether $(3.5.10)_4$ is also satisfied. Using a change of variable, we can write:

$$A_\sigma u(x) = \int_{\mathbb{R}} J(|\eta|)(u(x+\sigma\eta)-u(x))\,d\eta.$$

For small enough σ we expand $u(x+\sigma\eta)$ in a Taylor series about x, and obtain

$$\begin{aligned} A_\sigma u(x) &= \left(\int_{\mathbb{R}} J(|\eta|)\eta\,d\eta\right)u'(x)\sigma + \left(\int_{\mathbb{R}} J(|\eta|)\eta^2\,d\eta\right)u''(x)\sigma^2 + \mathcal{O}(\sigma^3) \\ &= \rho_2 u''(x)\sigma^2 + \mathcal{O}(\sigma^3). \end{aligned}$$

(To evaluate the first integral we used the positivity of J.) We see that if the initial data of (3.5.9) is such that

$$\|u_0\|_{C^2(\mathbb{R})} < \infty, \tag{3.5.20}$$

then the solution $u \in C^2(\mathbb{R})$, and $A_\sigma u = \mathcal{O}(\sigma^2)$ as $\sigma \to 0$. Thus, if the hypothesis $u_0 \in L^\infty(\Omega)$ in Theorem 3.28 is replaced by (3.5.20), then the result of this theorem holds. Note that A_σ given by (3.5.18) is in fact A_ϵ (with $\epsilon = \sigma$), and (3.5.19), (3.5.20) are exactly the extra-conditions used in Theorem 3.21 to prove non-coarsening of solutions of (3.3.1) for small enough ϵ. However, we believe that the restriction (3.5.20) used in Theorem 3.21 is a strong one, and the result holds for any $u_0 \in L^\infty(\Omega)$ that changes sign.

3.6 Truncations

The purpose of this section is to approximate the flow generated by

$$u_t = \gamma \int_{\mathbb{R}} J(|x-y|)[u(y)-u(x)]dy - f(u), \quad x \in \mathbb{R}, \tag{3.6.1}$$

by some flows which are obtained by taking Padé approximants. This equation is the $L^2(\mathbb{R})$ gradient flow of (3.2.3). As we can see later, one can derive formally the Ginzburg-Landau functional from (3.2.3) by expanding the term $(u(y)-u(x))$ in a Taylor series and truncating it at the first term. Difficulties arise if one tries to retain more than the leading term of the gradient expansion. In Subsection 3.6.2 we shall show that retaining an even number of terms one obtains an ill-posed problem. However, if we retain an odd number of terms we do get a well-posed problem on the positive semi-axis (such problems where considered in [8] and [10]), but it is not clear how to approximate the solution of (3.6.1) with a given initial data by solutions of the truncated gradient flow. A similar truncation technique of a nonlocal term has been used by Gourley in [56], where he studied the travelling front solutions of a nonlocal extension of the Fisher's equation.

In order to remove these difficulties we follow the idea in [90], and instead of polynomial approximations we use Padé approximants. The advantage of this method is that we find a new family of equations which are well-posed and we have the convergence property of solutions of this problems to the solution of the initial integro-differential equation (3.6.1).

3.6.1 Padé approximants

Padé approximants are rational approximations to functions defined as a formal power series expansion. Their power series expansion matches the series as far as possible, and are usually superior to Taylor series expansions when functions contain poles, because the use of rational functions allows them to be well-represented. Let f be a formal power series

$$f(z) = c_0 + c_1 z + c_2 z^2 + \cdots .$$

Definition 3.31 We call the $[p/q]$ *Padé approximant of* f, the rational function

$$R(z) = \frac{a_0 + a_1 z + a_2 z^2 + \cdots + a_p z^p}{b_0 + b_1 z + b_2 z^2 + \cdots + b_q z^q},$$

such that its power series expansion in ascending powers of z agrees with that of f up to the order of z^{p+q+1}, that is,

$$f(z) - r(z) = \mathcal{O}(z^{p+q+1}).$$

When it exists, the Padé approximant to any power series is unique.

For a thorough introduction in the Padé approximants theory and their properties one can consult, for example, the work of C. Brezinski [12].

If $\hat{u}(\xi)$ is the Fourier transform of $u(x)$, then the Fourier inversion formula is

$$u(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{u}(\xi) e^{ix\xi} d\xi. \tag{3.6.2}$$

Differentiating (3.6.2), one obtains

$$D^\alpha u(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \xi^\alpha \hat{u}(\xi) e^{ix\xi} d\xi, \quad \alpha = 1, 2, \ldots.$$

where $D^\alpha = \dfrac{1}{i^\alpha} \dfrac{\partial^\alpha}{\partial x^\alpha}$. Using the properties of the Fourier transform, if we apply to $u(x)$ the differential operator

$$p(D) = \sum_{|\alpha| \leq k} a_\alpha D^\alpha, \quad (a_\alpha \in \mathbb{R}),$$

we get

$$p(D)u(x) = \frac{1}{2\pi} \int_{\mathbb{R}} p(\xi) \hat{u}(\xi) e^{ix\xi} d\xi,$$

where

$$p(\xi) = \sum_{|\alpha| \leq k} a_\alpha \xi^\alpha.$$

The polynomial $p(\xi)$ is called the *symbol* of the differential operator $p(D)$. In the next subsections we shall denote the symbol of an operator A by $\mathcal{S}(A)$.

3.6.2 The truncation scheme

We aim to derive the truncated gradient flows of (3.2.3) by expanding in Taylor series the term $(u(y)-u(x))$, and then truncate to some order the new expression. Since we are expanding the interface part of the free energy, we shall omit the bulk energy part in the computations below. We denote by $L(u)$ the linear part of the free energy, that is

$$L(u) = \frac{\gamma}{4}\int_{\mathbb{R}}\int_{\mathbb{R}} J(|x-y|)(u(y)-u(x))^2\,dy\,dx.$$

In this section we shall use the notation $D^k u$ for the k-th derivative of u. Setting $x = \xi - \eta$ and $y = \xi - \eta$, and then expanding $u(x) = u(\xi+\eta)$ and $u(y) = u(\xi-\eta)$ about ξ, we have formally

$$\begin{aligned} L(u) &= \frac{\gamma}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} J(2|\eta|)[u(\xi-\eta)-u(\xi+\eta)]^2\,d\eta\,d\xi \\ &= 2\gamma\int_{\mathbb{R}}\int_{\mathbb{R}} J(2|\eta|)\left[\sum_{k=1}^{\infty}\frac{\eta^{2k-1}}{(2k-1)!}D^{2k-1}u(\xi)\right]^2 d\xi d\eta \\ &= 2\gamma\int_{\mathbb{R}} J(2|\eta|)\sum_{k=1}^{\infty}\frac{\eta^{2k}}{(2k)!}\left[\int_{\mathbb{R}}\sum_{i=1}^{k} C_{2k}^{2i-1}D^{2i-1}u(\xi)D^{2k-2i+1}u(\xi)\,d\xi\right]d\eta, \quad (3.6.3) \end{aligned}$$

where C_{2k}^{2i-1} is defined by

$$C_{2k}^{2i-1} = \frac{(2k)!}{(2i-1)!(2k-2i+1)!}, \qquad k = 1,2,\ldots;\ \ i = 1,2,\ldots,k.$$

We now truncate to the *nth*-order the last expression of $L(u)$ and write

$$L_n(u) = 2\gamma\int_{\mathbb{R}} J(2|\eta|)\sum_{k=1}^{n}\frac{\eta^{2k}}{(2k)!}\left[\int_{\mathbb{R}}\sum_{i=1}^{k} C_{2k}^{2i-1}D^{2i-1}u(\xi)D^{2k-2i+1}u(\xi)\,d\xi\right]d\eta.$$

Again, proceeding formally we compute the $L^2(\Omega)$ gradient flow of the truncated free energy $E_n(u)$, where

$$E_n(u) = L_n(u) + \int_{\mathbb{R}} F(u(x))dx.$$

We have

$$
\begin{aligned}
&< \frac{\delta E_n(u)}{\delta u}, v > = \\
&\quad = \frac{d}{d\theta} E_n(u+\theta v)|_{\theta=0} \\
&\quad = 2\gamma \int_{\mathbb{R}} J(2|\eta|) \sum_{k=1}^{n} \frac{\eta^{2k}}{(2k)!} \{ \sum_{i=1}^{k} C_{2k}^{2i-1} \int_{\mathbb{R}} [D^{2i-1}u(\xi) D^{2k-2i+1} v(\xi) + \\
&\qquad + D^{2i-1} v(\xi) D^{2k-2i+1} u(\xi)] d\xi \} d\eta + \int_{\mathbb{R}} f(u(\xi)) v(\xi)\, d\xi \\
&= 2\gamma \int_{\mathbb{R}} J(2|\eta|) \sum_{k=1}^{n} \frac{\eta^{2k}}{(2k)!} \{ \sum_{i=1}^{k} C_{2k}^{2i-1} \int_{\mathbb{R}} [(-1)^{2k-2i+1} D^{2k} u(\xi) + \\
&\qquad + (-1)^{2i-1} D^{2k} u(\xi)] v(\xi) d\xi \} d\eta + \int_{\mathbb{R}} f(u(\xi)) v(\xi)\, d\xi \qquad (3.6.4) \\
&= -\gamma \int_{\mathbb{R}} \left\{ \sum_{k=1}^{n} \left[\frac{2^{2k+1}}{(2k)!} \int_{\mathbb{R}} J(2|\eta|) \eta^{2k} d\eta \right] D^{2k} u(\xi) - f(u(\xi)) \right\} v(\xi) d\xi \\
&= -\gamma \int_{\mathbb{R}} \left\{ \sum_{k=1}^{n} \rho_{2k} D^{2k} u(\xi) - f(u(\xi)) \right\} v(\xi) d\xi, \quad \text{for all } v \in L^2(\Omega),
\end{aligned}
$$

where by ρ_{2k} we have defined the non-negative quantities

$$
\begin{aligned}
\rho_{2k} &= \frac{2^{2k+1}}{(2k)!} \int_{\mathbb{R}} J(2|\eta|) \eta^{2k} d\eta, \\
&= \frac{1}{(2k)!} \int_{\mathbb{R}} J(|z|) z^{2k}\, dz, \qquad k = 1, 2, \ldots \qquad (3.6.5)
\end{aligned}
$$

Note that in (3.6.4) we used integration by parts, and homogeneous boundary conditions for the derivatives of u of any order.

For the infinite series to be at least formally defined we must assume that all the moments ρ_{2k} of $J(\cdot)$ are finite.

Thus, the $L^2(\Omega)$ gradient flow is

$$
\frac{\partial u}{\partial t}(x,\, t) = \gamma \sum_{k=1}^{n} \rho_{2k} D^{2k} u(x,\, t) - f(u(x,\, t)), \qquad x \in \mathbb{R}. \qquad (3.6.6)
$$

Remark 3.32 Note that we can also derive formally the L^2-gradient flow of the expanded free energy (3.6.3). This is

$$
\frac{\partial u}{\partial t} = \gamma \sum_{k=1}^{\infty} \rho_{2k} D^{2k} u - f(u), \qquad (3.6.7)
$$

which can be written in the form

$$u_t = \gamma \int_{\mathbb{R}} J(|z|)[\cosh(zD)]u(x)\,dz - f(u), \quad x \in \mathbb{R},$$

which is reminiscent of equations derived in [89]. By $\cosh(zD)$ we have defined the differential operator

$$\cosh(zD)(u) = \frac{1}{(2k)!}\sum_{k=1}^{\infty} z^{2k} D^{2k} u.$$

The symbol of this operator is then

$$\cos(z\xi) = \frac{1}{(2k)!}\sum_{k=1}^{\infty} (-1)^k z^{2k}\xi^{2k}.$$

Therefore, if A denotes the bounded integral operator

$$Au(x) = \int_{\mathbb{R}} J(|x-y|)(u(y)-u(x))\,dy, \quad x \in \mathbb{R}, \tag{3.6.8}$$

then the symbol of A is

$$\mathcal{S}(A)(\xi) = \int_{\mathbb{R}} J(|z|)(\cos(z\xi)-1)\,dz. \tag{3.6.9}$$

This discussion suggests another way (also formal) of obtaining the equation (3.6.6). One can expand $(\cos(z\xi)-1)$ in Taylor series and then integrate term by term, to get the series

$$\sum_{k=1}^{\infty} \rho_{2k} D^{2k} u. \tag{3.6.10}$$

Finally, we truncate the series to the *nth* order and obtain the differential operator in (3.6.6).

Let us now define the operator

$$\widetilde{A}_n u = \sum_{k=1}^{n} \rho_{2k} D^{2k} u, \quad n \in \mathbb{N},$$

and for each $n \in \mathbb{N}$ consider the following initial value problem in $L^2(\mathbb{R})$:

$$(\widetilde{\mathcal{P}}_n) \quad \begin{cases} u_t = \gamma \widetilde{A}_n u - f(u), \quad (x,t) \in \mathbb{R} \times (0,\infty). \\ u(0) = u_0, \end{cases} \tag{3.6.11}$$

We can make the following discussion regarding the well-posedness of these problems. If $J(\cdot) \geq 0$, then the operator $(-1)^{n+1}\widetilde{A_n}$ is elliptic and so, for n even these problems are not well-posed in positive time, and for n odd the problems $(\widetilde{\mathcal{P}}_n)$ are not well-posed in negative time. The natural question that can be raised here is: which is the right setting (if at all) in which these initial value problems are well-posed for all the values of n?

In order to answer this question, we suggest approximating the flow generated by (3.6.1) by taking operator Padé approximants of $(\widetilde{\mathcal{P}}_n)$. Thus, for each n we aim to derive an equation that generates a semi-flow. Let $\mathcal{S}(\widetilde{A}_{2n})$ be the symbol of the operator $\widetilde{A}_{2n}$ (a polynomial of degree $4n$). If

$$\frac{q_{2n}}{r_{2n}} \text{ is the } [2n/2n] \text{ Padé approximant of } \mathcal{S}(\widetilde{A}_{2n}),$$

(where p_{2n}, q_{2n} are polynomials of degree $2n$), then we consider the differential operators R_n and Q_n of order $2n$, such that

$$\mathcal{S}(Q_n) = q_{2n} \quad \text{and} \quad \mathcal{S}(R_n) = r_{2n}.$$

In this way, the truncation to degree $2n$ of the symbol of $A_{2n}R_n$ is the symbol of Q_n. For each $n \in \mathbb{N}$ we define the operator

$$A_n = Q_n R_n^{-1}$$

acting on $L^2(\mathbb{R})$, which is the $[2n/2n]$ Padé approximant of $\sum_{k=1}^{\infty} \rho_{2k} D^{2k} u$. Thus, instead of the family of problems $(\widetilde{\mathcal{P}}_n)$ we can the consider the following evolutionary problems:

$$(\mathcal{P}_n) \quad \begin{cases} u_t = \gamma A_n u - f(u), \quad (x,t) \in \mathbb{R} \times (0,\infty), \\ \\ u(0) = u_0. \end{cases} \tag{3.6.12}$$

Remark 3.33 From the definition of A_n we have that

$$\mathcal{S}(A_n)(\xi) - \mathcal{S}(A)(\xi) = \mathcal{O}(\xi^{2n+1}). \tag{3.6.13}$$

The symbol $\mathcal{S}(A)$ of A is a bounded function of ξ even if $J(\cdot)$ is not always positive. Indeed,

$$|\mathcal{S}(A)(\xi)| \leq \int_{\mathbb{R}} |J(|\xi|)||\cos(z\xi) - 1|\, d\xi \leq 2, \text{ for all } \xi \in \mathbb{R}.$$

As we shall see in the next subsection, if the problem $(\widetilde{\mathcal{P}}_n)$ can be ill-posed, the problems $(\mathcal{P}_n)$ derived by using Padé approximants will always be well-posed.

Remark 3.34 The differential operators satisfy the commutativity property

$$R_n Q_n = Q_n R_n$$

on smooth enough functions (usual property of differential operators with constant coefficients), and using this we can write $(3.6.12)_1$ in the form

$$R_n(u_t + f(u)) = Q_n u, \quad (x,t) \in \mathbb{R} \times (0,\infty), \ \ n \in \mathbb{N}. \tag{3.6.14}$$

There is a problem with the equation written in this form: in order to study (3.6.14) one also needs boundary conditions to be set, which are not required in the case of the initial value problem (3.6.12).

However, if we consider the particular case $n = 1$, then (3.6.14) turns out to be the following equation

$$\left(\rho_2 I - \rho_4 \frac{\partial^2}{\partial x^2}\right)(u_t + f(u)) = \gamma \rho_2^2 \frac{\partial^2 u}{\partial x^2}, \quad x \in \mathbb{R}, \tag{3.6.15}$$

which must be considered together with appropriate boundary conditions, where I is the identity operator and ρ_2, ρ_4 are given by (3.6.5).

3.6.3 Well-posedness and convergence

For each $n \in \mathbb{N}$, we aim to derive a semigroup theory approach for the problem $(\mathcal{P}_n)$ and show that the family of solutions we obtain converge to the solution of the initial integro-differential problem. We start by the following lemma:

Lemma 3.35 *A_n, $n \in \mathbb{N}$, are bounded linear operators on $L^2(\mathbb{R})$.*

Proof. Clearly, A_n is a linear operator for each $n \in \mathbb{N}$, since both Q_n and R_n are linear and the inverse of a linear operator is linear. From (3.6.13) and the fact that the symbol of A, given by (3.6.9), is a bounded function from $\mathbb{R}$ into $\mathbb{R}$, we get that the symbols of A_n, $n \in \mathbb{N}$, are bounded. Therefore, by applying the Plancherel formula in the form

$$\|A_n u\|_2 = \|\widehat{A_n u}\|_2 = \|\mathcal{S}(A_n)\widehat{u}\|_2,$$

where $\widehat{u}$ is the Fourier transform of $u \in L^2(\mathbb{R})$, we see that A_n are bounded operators in $L^2(\mathbb{R})$. □

It is also possible to prove the boundedness of A_n in the L^∞-norm, which would allow us to derive the semigroup theory approach in $L^\infty(\mathbb{R})$. We have the following lemma:

Lemma 3.36 *A_n, $n \in \mathbb{N}$, are bounded linear operators on $L^\infty(\mathbb{R})$.*

To prove this result we shall work with the Schwartz space of *tempered distributions on* $\mathbb{R}$ (see [93] for an introduction). Recall that a *distribution* $T \in \mathcal{D}'(\mathbb{R})$ is a continuous linear functional on $\mathcal{D}(\mathbb{R})$. If we define the space

$$\mathcal{S}(\mathbb{R}) = \{u \in C^\infty(\mathbb{R}) : \text{ for all } \alpha, \beta \in \mathbb{N}, \sup_{x \in \mathbb{R}} |x^\alpha u^{(\beta)}(x)| < \infty\},$$

then a *tempered distribution on* $\mathbb{R}$ is a continuous linear functional on $\mathcal{S}(\mathbb{R})$, that is, a continuous linear map from $\mathcal{S}(\mathbb{R})$ to $\mathbb{R}$. The space of tempered distributions is denoted by $\mathcal{S}'(\mathbb{R})$. Note that we have $\mathcal{D}(\mathbb{R}) \subset \mathcal{S}(\mathbb{R}) \subset \mathcal{S}'(\mathbb{R}) \subset \mathcal{D}'(\mathbb{R})$. If $u \in \mathcal{S}(\mathbb{R})$, then the Fourier transform of u is the function defined by

$$\mathcal{F}u(\xi) \equiv \hat{u}(\xi) = \int_{\mathbb{R}} e^{-ix\xi} u(x) dx, \text{ for all } \xi \in \mathbb{R}. \tag{3.6.16}$$

The Fourier transform can be extended to $\mathcal{S}'(\mathbb{R})$ as follows: for $T \in \mathcal{S}'(\mathbb{R})$, define

$$< \hat{T}, \phi > \equiv < T, \hat{\phi} >, \text{ for all } \phi \in \mathcal{S}(\mathbb{R}). \tag{3.6.17}$$

For a function $u \in L^1_{loc}(\mathbb{R})$ there is a natural distribution, also denoted by u, and sometimes called *a generalized function*, defined by

$$u(\phi) = \int_{\mathbb{R}} u(\xi)\phi(\xi) d\xi, \text{ for all } \phi \in \mathcal{D}(\mathbb{R}).$$

We can easily see that for a function $u \in L^\infty(\mathbb{R}) \subset L^1_{loc}(\mathbb{R})$, the corresponding generalized function u is a tempered distribution, and thus its Fourier transform is defined. With all these in mind we start now proving Lemma 3.36.

Proof. (*Lemma* 3.36) Since $A_n u = Q_n R_n^{-1} u$, then the theorem is proved if the following two inequalities hold:

- If $u \in L^\infty(\mathbb{R})$ and z is a weak solution of $R_n z = u$ in the distribution sense, then $z \in W^{2n,\infty}(\mathbb{R})$ and

$$\|z\|_{W^{2n,\infty}(\mathbb{R})} \leq C_{1n}\|u\|_{L^\infty(\mathbb{R})}. \tag{3.6.18}$$

- For $z \in W^{2n,\infty}(\mathbb{R})$, we have

$$\|Q_n z\|_{L^\infty(\mathbb{R})} \leq C_{2n}\|z\|_{W^{2n,\infty}(\mathbb{R})}. \tag{3.6.19}$$

Recall that R_n has the form $R_n z = \sum_{k=0}^{n} a_{2k} D^{2k} z$, where a_{2k} are some real constants. Since $\mathcal{S}(A_n)$ is bounded, we can suppose that

$$P(\xi) := \mathcal{S}(R_n)(\xi) = \sum_{k=0}^{n} (-1)^k a_{2k} \xi^{2k} > 0, \text{ for all } \xi \in \mathbb{R}.$$

Let us now prove the first inequality. The function z is a weak solution of $R_n z = u$ if

$$R_n z = u, \quad \text{in } \mathcal{D}'(\mathbb{R}), \tag{3.6.20}$$

that is,

$$\int_{\mathbb{R}} R_n z(\xi)\phi(\xi)d\xi = \int_{\mathbb{R}} u(\xi)\phi(\xi)d\xi, \quad \text{for all } \phi \in \mathcal{D}(\mathbb{R}).$$

As we discussed earlier, because $u \in L^\infty(\mathbb{R})$, the corresponding generalized function, that is u, is in $\mathcal{S}'(\mathbb{R}) \subset \mathcal{D}'(\mathbb{R})$, hence its Fourier transform is defined. Taking the Fourier transform in (3.6.20), we get

$$\widehat{R_n z}(\xi) = \hat{u}(\xi), \text{ for all } \xi \in \mathbb{R}, \tag{3.6.21}$$

where this equation is also considered in $\mathcal{D}'(\mathbb{R})$, and it is equivalent to

$$P(\xi)\hat{z}(\xi) = \hat{u}(\xi), \text{ for all } \xi \in \mathbb{R}. \tag{3.6.22}$$

Since the symbol of R_n is positive, then for all $k = 0, 1, \ldots, n$, there exists some positive constant α_k, such that

$$\alpha_k \xi^{2k} \hat{z}(\xi) \leq P(\xi)\hat{z}(\xi) = \hat{u}(\xi), \text{ for all } \xi \in \mathbb{R}, \tag{3.6.23}$$

and thus

$$\alpha_k |\widehat{D^{2k} z}(\xi)| \leq |\hat{u}(\xi)|, \text{ for all } \xi,$$

which implies

$$\begin{aligned} |\int_{\mathbb{R}} D^{2k}z(\xi)\hat{\phi}(\xi)\,d\xi| &= |\int_{\mathbb{R}} \widehat{D^{2k}z}(\xi)\phi(\xi)\,d\xi| \\ &\leq C_k|\int_{\mathbb{R}} \hat{u}(\xi)\phi(\xi)\,d\xi| \\ &\leq C_k|\int_{\mathbb{R}} u(\xi)\hat{\phi}(\xi)\,d\xi| \\ &\leq C_k\|u\|_{L^\infty(\mathbb{R})}\|\hat{\phi}\|_{L^1(\mathbb{R})}, \qquad k=1,2,\ldots,n \quad (3.6.24) \end{aligned}$$

for all $\phi \in \mathcal{D}(\mathbb{R})$, where C_k are some positive constants. From (3.6.24) we get that $D^{2k}z$ are in $L^\infty(\mathbb{R})$ and

$$\|D^{2k}z\|_{L^\infty(\mathbb{R})} \leq C_k\|u\|_{L^\infty(\mathbb{R})}, \text{ for all } k=1,2,\ldots,n.$$

Since the norm in $W^{2n,\infty}(\mathbb{R})$ is given by

$$\|z\|_{W^{2n,\infty}(\mathbb{R})} = \max_{0\leq k\leq 2n} \|D^k z\|_{L^\infty(\mathbb{R})},$$

from the previous inequalities we can conclude that

$$z \in W^{2n,\infty}(\mathbb{R}) \text{ and } \|z\|_{W^{2n,\infty}(\mathbb{R})} \leq C_{1n}\|u\|_{L^\infty(\mathbb{R})}.$$

Here $C_{1n} = \max\limits_{0\leq k\leq 2n} C_k$. In order to prove (3.6.19) let us note that Q_n has the form

$$Q_n z = \sum_{k=0}^{n} b_{2k} D^{2k} z$$

where b_{2k} are some real constants. Then (3.6.19) results from

$$\begin{aligned} \|Q_n z\|_{L^\infty(\mathbb{R})} &\leq \sum_{k=0}^{n} |b_{2k}| \|D^{2k}z\|_{L^\infty(\mathbb{R})} \\ &\leq (\sum_{k=0}^{n} |b_{2k}|) \max_{0\leq k\leq n} \|D^{2k}z\|_{L^\infty(\mathbb{R})} \\ &= C_{2n} \max_{0\leq k\leq n} \|D^{2k}z\|_{L^\infty(\mathbb{R})} \\ &= C_{2n}\|z\|_{W^{2n,\infty}(\mathbb{R})}. \end{aligned}$$

□

Because $L^2(\mathbb{R})$ is a Hilbert space, and thus easier to use for our purposes, we shall continue our investigations in this space. We restrict ourselves to the space

$\{u \in L^2(\mathbb{R});\ \text{supp}\ u = \Omega\}$, where Ω is a bounded domain in $\mathbb{R}$, and for each $n \in \mathbb{N}$ we study the following initial value problem

$$\begin{cases} u_t = \gamma A_n u - f(u), \quad (x,t) \in \Omega \times (0,\infty), \\ u(0) = u_0. \end{cases} \tag{3.6.25}$$

We would like to prove that this problem generates a flow on $L^2(\Omega)$, a space in which the steady state patterns of interest lie. We make the following assumptions:

$(\mathcal{A}_1)$ $\quad J \in L^1(\mathbb{R})$ and $\int_{\mathbb{R}} J(x)e^x dx < \infty$;

$(\mathcal{A}_2)$ $\quad$ the function $f : L^2(\Omega) \to L^2(\Omega)$ is locally Lipschitz continuous.

Note that $(\mathcal{A}_1)$ assures that all the coefficients ρ_{2k}, $k \in \mathbb{N}$, are defined and, implicitly, the operator A_n is defined for each $n \in \mathbb{N}$.

Definition 3.37 For a fixed $n \in \mathbb{N}$, we say that a function $u : [0,T) \to L^2(\Omega)$ is a *(classical) solution* of (3.6.25) on $[0,T)$ if u is continuous on $[0,T)$, continuously differentiable on $(0,T)$, and (3.6.25) is satisfied on $[0,T)$.

We have the following existence and uniqueness result:

Theorem 3.38 *Suppose that the hypotheses $(\mathcal{A}_1)$ and $(\mathcal{A}_2)$ are satisfied, and the function f has the additional property*

$$\liminf_{\|u\|_2 \to \infty} \frac{f(u)}{u} \geq 0. \tag{3.6.26}$$

For each $n \in \mathbb{N}$, if $u_0 \in L^2(\Omega)$, then the initial value problem (3.6.25) has a unique global solution $u_n \in C([0,\infty); L^2(\Omega))$. Moreover, for each $n \in \mathbb{N}$ the mapping $u_0 \to u_n$ is continuous in $L^2(\Omega)$.

Proof. We choose an arbitrary $n_0 \in \mathbb{N}$, and then fix it. Since A_{n_0} is a bounded operator on $L^2(\mathbb{R})$ and $supp\, u = \Omega$, then A_{n_0} is bounded on $L^2(\Omega)$, and it is the infinitesimal generator of a uniformly continuous semigroup $\{S_{n_0}(t),\ t \geq 0\}$. For an initial condition $u_0 \in D(A_{n_0}) = L^2(\Omega)$, the theory of Lipschitz perturbations of linear evolution equations (see Pazy [84]) assures the existence and uniqueness

of a local solution $u_{n_0}(x,t,u_0)$, defined on a maximal interval of existence $[0,\tau^{n_0})$ (with τ^{n_0} depending on $\|u_0\|$), and also the continuity of u_{n_0} with respect to the initial condition. Moreover, if $\tau^{n_0} < \infty$, then $\lim_{t\nearrow\tau^{n_0}} \|u(t)\| = \infty$. We would like to show that solutions are defined for $t \geq 0$, so we need to find an *a priori* bound of $u_{n_0}(t)$ in $L^2(\Omega)$. Since the operator A_{n_0} is bounded, there is a positive constant M_{n_0} such that

$$< A_{n_0}u,\, u > \leq\ M_{n_0}\|u\|^2, \qquad \text{for all } u \in L^2(\Omega).$$

The condition (3.6.26) implies that for any $\mu > 0$ there is a positive constant C_μ such that

$$\begin{aligned} - < f(u),\, u > &= -\int_\Omega [\frac{f(u)}{u} - \mu]u^2 dx - \mu\|u\|^2 \\ &\leq C_\mu - \mu\|u\|^2. \end{aligned} \tag{3.6.27}$$

Taking the inner product of $(3.6.25)_1$ with u, and using (3.6.27) with $\mu > \gamma M_{n_0}$, then we have

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|u(t)\|^2 &= \gamma < A_{n_0}u(t), u(t) > - < f(u(t)), u(t) > \\ &\leq (\gamma M_{n_0} - \mu)\|u(t)\|^2 + C_\mu, \quad \text{for all } u \in L^2(\Omega), \end{aligned}$$

which, by Gronwall's inequality, implies that

$$\begin{aligned} \|u(t)\|^2 &\leq \|u_0\|^2 \exp(-Ct) + \frac{C_\mu}{C}[1 - \exp(-Ct)] \\ &\leq \max(\|u_0\|^2,\, \frac{C_\mu}{C}), \quad \text{for } 0 \leq t < \tau^{n_0}, \end{aligned} \tag{3.6.28}$$

where $C = 2(\mu - \gamma M_{n_0}) > 0$. In particular, we obtain the boundedness of $u_{n_0}(t)$ in $L^2(\Omega)$ and thus, the solution $u_{n_0}(x,t;u_0)$ is globally defined on $L^2(\Omega)$. □

Remark 3.39 For each $n \in \mathbb{N}$, we denote by $u_n(x,t;u_0)$ the solution to (3.6.25). Then, for each $n \in \mathbb{N}$, the solution operators $\{T_n(t) : L^2(\Omega) \to L^2(\Omega),\ t \geq 0\}$, defined by

$$T_n(t)u_0 = u_n(t;u_0), \quad t \geq 0,$$

form a continuous semigroup of bounded nonlinear operators.

The inequality (3.6.28) implies that for each $n \in \mathbb{N}$,

$$\limsup_{t\to\infty} \|u_n(t)\|^2 \leq \frac{C_\mu}{C}.$$

Setting $\rho_0 = (C_\mu/C)^{1/2}$, we see that any ball of $L^2(\Omega)$, centered at 0 of radius $\rho \geq \rho_0$, is positively invariant for the semigroup $\{T_n(t)\}_{t\geq 0}$. Also, it can be easily deduced from (3.6.28) that any ball $\mathcal{B}(0, \rho)$, $\rho \geq \rho_0$, is absorbing in $L^2(\Omega)$. Indeed, if we fix ρ arbitrarily, such that $\rho \geq \rho_0$, and let $\mathcal{B}$ be any bounded set of $L^2(\Omega)$ included in the ball $B(0, R)$ for some $R > 0$, then we get from (3.6.28) that

$$T_n(t)\mathcal{B} \subset \mathcal{B}(0, \rho), \quad \text{for } t \geq t_0 = t_0(\mathcal{B}, \rho),$$

with

$$t_0 = \frac{1}{C} \ln \frac{R^2}{\rho^2 - \rho_0^2}.$$

Let us denote by $u(x, t; u_0)$ the solution to (3.6.1) with $u(x, 0) = u_0$, and by $\{T(t) : L^2(\Omega) \to L^2(\Omega),\ t \geq 0\}$ the continuous semigroup of bounded nonlinear operators generated by (3.6.1). We would like now to show that solutions to (3.6.25) with $u(x, 0)$ given, converge in the $L^2(\Omega)$ norm to solutions to (3.6.1) with the same initial data, as $n \to \infty$. To prove such a result we need the following lemma:

Lemma 3.40 *If X is a Banach space and the sequence $\{w_n, n \in \mathbb{N}\} \subset C([0, t]; X)$ converges to w in the sense of the norm of $C([0, t]; X)$, then*

$$\lim_{n\to\infty} \int_0^t w_n(r)dr = \int_0^t w(r)dr, \quad \text{in the } X \text{ norm.} \tag{3.6.29}$$

Proof. See [11], Theorem 3.3. □

We can now prove the following approximation result:

Theorem 3.41 *For every $u_0 \in L^2(\Omega)$ and each $t > 0$, we have that*

$$\|u_n(t; u_0) - u(t; u_0)\|_2 \to 0, \ \text{as } n \to \infty. \tag{3.6.30}$$

Proof. Denote by $\{S(t);\, t \geq 0\}$ and $\{S_n(t);\, t \geq 0\}$ the linear continuous semigroups generated by the linear continuous operators A and A_n $(n \in \mathbb{N})$, respectively. Since these semigroups are bounded, we can find some positive constants M and $M_n\,(n \in \mathbb{N})$ so that $\|S(t)\|_2 \leq M$ and $\|S_n(t)\|_2 \leq M_n\,(n \in \mathbb{N})$. If we let $g(u) = -f(u)$, then the solutions of (3.6.1) and, respectively, (3.6.25) can be written in the form

$$u(t;\, u_0) = S(t)u_0 + \int_0^t S(t-s)g(u(s))\,ds, \quad t \geq 0,$$

and

$$u_n(t;\, u_0) = S_n(t)u_0 + \int_0^t S_n(t-s)g(u_n(s))\,ds, \quad t \geq 0,\ n \in \mathbb{N}.$$

The function g is locally Lipschitz continuous. Hence for every positive constant c there is a constant $L_c > 0$ such that

$$\|g(u) - g(v)\|_2 \leq L_c\|u - v\|_2$$

holds for all $u,\, v \in L^2(\Omega)$ with $\|u\|_2 \leq c$, $\|v\|_2 \leq c$. Since S and $S_n, n \in \mathbb{N}$, are bounded semigroups on $L^2(\Omega)$, we can choose $c > 0$ to be their common L^2-upper bound. Thus, abbreviating $u(t;\, u_0)$ and $u_n(t;\, u_0)$ to $u(t)$ and $u_n(t)$ respectively, it follows that, for all $t > 0$,

$$\begin{aligned}
\|u_n(t) - u(t)\|_2 \leq & \\
&\leq \|S_n(t)u_0 - S(t)u_0\|_2 + \int_0^t \|S_n(t-s)g(u_n(s)) - S(t-s)g(u(s))\|_2 ds \\
&\leq \|[S_n(t) - S(t)]u_0\|_2 + \int_0^t \|[S_n(t-s) - S(t-s)]g(u(s))\|_2 ds \\
&\quad + \int_0^t \|S_n(t-s)g(u_n(s)) - S_n(t-s)g(u(s))\|_2 ds \\
&\leq \|[S_n(t) - S(t)]u_0\|_2 + \int_0^t \|[S_n(t-s) - S(t-s)]g(u(s))\|_2 ds \\
&\quad + M_n L_c \int_0^t \|u_n(s) - u(s)\|_2 ds,
\end{aligned}$$

for all $n \in \mathbb{N}$. We can rewrite the last inequality as

$$\begin{aligned}
\frac{d}{dt}\{e^{-M_n L_c t} \int_0^t \|u_n(s) - u(s)\|_2 ds\} \leq e^{-M_n L_c t}\{ \|\,[S_n(t) - S(t)]u_0\|_2 + \\
+ \int_0^t \|[S_n(t-s) - S(t-s)]g(u(s))\|_2 ds\,\},
\end{aligned}$$

for all $n \in \mathbb{N}$. Then, using the above Lemma, the convergence (3.6.30) is proved if for all $h \in L^2(\Omega)$ we have

$$\|S_n(t)h - S(t)h\|_2 \to 0, \text{ as } n \to \infty. \tag{3.6.31}$$

By the Trotter approximation theorem (see [84]), in order to have (3.6.31) it suffices to prove the following convergence in the $L^2(\Omega)$ norm, for the corresponding resolvents:

$$\text{for every } h \in L^2(\Omega) \text{ and some } \lambda > 0,$$
$$R(\lambda, A_n)h \to R(\lambda, A)h \text{ as } n \to \infty, \tag{3.6.32}$$

where $R(\lambda, A) = (\lambda I - A)^{-1}$ and $R(\lambda, A_n) = (\lambda I - A_n)^{-1}$, $n \in \mathbb{N}$. Since A and A_n $(n \in \mathbb{N})$ are infinitesimal generators of the uniformly continuous semigroups $\{S(t), t \geq 0\}$ and, respectively, $\{S_n(t), t \geq 0\}$ $(n \in \mathbb{N})$, the Hille-Yosida theorem implies that the resolvent sets $\rho(A)$ and $\rho(A_n)$ $(n \in \mathbb{N})$ contain $(0, \infty)$ and

$$\|R(\lambda, A)\|_2 \leq M/\lambda, \qquad \|R(\lambda, A_n)\|_2 \leq M_n/\lambda \quad \text{for } \lambda > 0, \quad n = 1, 2, \ldots$$

Then, for all $h \in L^2(\Omega)$, we have :

$$\begin{aligned}\|R(\lambda, A_n)h - R(\lambda, A)h\|_2 &= \|R(\lambda, A_n)\{(\lambda I - A) - (\lambda I - A_n)\}R(\lambda, A)h\|_2 \\ &= \|R(\lambda, A_n)[A_n - A]R(\lambda, A)h\|_2 \\ &\leq \frac{M_n}{\lambda}\| [A_n - A]R(\lambda, A)h \|_2, \qquad \lambda > 0. \end{aligned} \tag{3.6.33}$$

On the other hand, for each $n \in \mathbb{N}$ the symbol $\mathcal{S}(A_n)$ is the $[2n/2n]$ Padé approximant of $\mathcal{S}(A)$. This fact and the Plancherel formula implies

$$\begin{aligned}\|(A_n - A)\xi\|_2 &= \| \mathcal{F}[(A_n - A)\xi] \|_2 \\ &= \|[\mathcal{S}(A_n) - \mathcal{S}(A)]\mathcal{F}\xi\|_2 \\ &\leq \|\mathcal{S}(A_n) - \mathcal{S}(A)\|_2\|\xi\|_2 \overset{n\to\infty}{\longrightarrow} 0, \quad \text{for all } \xi \in L^2(\Omega), \end{aligned} \tag{3.6.34}$$

where $\mathcal{F}\xi$ denotes the Fourier transform. From (3.6.34) and (3.6.33) we get (3.6.32), and this ends the proof. □

Remark 3.42 Using a truncation scheme, we can easily derive the Cahn-Hilliard equation and the viscous diffusion equation (2.2.23) (see also [82]) from the conserved order parameter version of (3.6.1), which is

$$u_t = -\gamma A \circ Au - Af(u), \quad (x, t) \in \mathbb{R} \times (0, \infty), \tag{3.6.35}$$

where A is the operator (3.6.8) (the equation (3.6.35) will be discussed in Chapter 4). Indeed, after we change the variables and expand in Taylor series, we obtain formally

$$u_t = -\gamma A_\infty \circ A_\infty u + A_\infty f(u), \tag{3.6.36}$$

where A_∞ denotes the operator (3.6.10). Truncating A_∞ at the first term yields the Cahn-Hilliard equation written in the one dimensional form

$$u_t = \frac{\partial^2}{\partial x^2}\left(f(u) - \gamma\rho_2 \frac{\partial^2 u}{\partial x^2}\right), \quad (x, t) \in \mathbb{R} \times (0, \infty).$$

Furthermore, if we set $\gamma = 0$ and take the [2/2] Padé approximant, we obtain the equation

$$\left(\rho_2 I - \rho_4 \frac{\partial^2}{\partial x^2}\right) u_t = \gamma\rho_2^2 \frac{\partial^2}{\partial x^2} f(u), \quad (x, t) \in \mathbb{R} \times (0, \infty),$$

which was derived and analyzed by A. Novick-Cohen and R. L. Pego in [82] (see also Section 2.2.4).

3.7 Numerical analysis

In this section we outline a numerical approximation method, using which we carry out experiments in order to verify and illustrate the results of Section 3.5.

3.7.1 Numerical approximation

We aim to approximate the equation (3.3.1) in one space dimension by a system of ordinary differential equations using discretisation in space. We take, for

simplicity, $\Omega = [0, 1]$ and $f(u) = u^3 - u$. The equation (3.3.1) becomes

$$u_t = \frac{\gamma}{\varepsilon}\left(\int_0^1 J(\frac{|x-y|}{\varepsilon})u(y)dy - u(x)\int_0^1 J(\frac{|x-y|}{\varepsilon})dy\right) + u - u^3, \quad x \in (0, 1). \tag{3.7.1}$$

We denote by $\bar{J}_\varepsilon(x) = J(\frac{x}{\varepsilon})$. Let us partition the interval [0, 1] by the equally spaced points

$$0 = x_0 < x_1 < \cdots < x_{i-1} < x_i < \cdots < x_N = 1,$$

where $x_i = i\Delta x$ and $\Delta x = 1/N$. We approximate the solution of (3.7.1) by functions that are piecewise constant in space,

$$u(x, t) \approx u_i(t)\chi_{(x_{i-1}, x_i)}(x), \quad \text{for all } x \in (0, 1).$$

For each $i = 1, 2, \ldots, N$, we take $x = x_{i-\frac{1}{2}}$ $(= \dfrac{x_{i-1} + x_i}{2})$ in (3.7.1). We get

$$\frac{du_i}{dt} = \frac{\gamma}{\varepsilon}\left(\int_0^1 \bar{J}_\varepsilon(|x_{i-\frac{1}{2}} - y|)u_k\chi_{(x_{k-1}, x_k)}(y)dy - u_i\int_0^1 \bar{J}_\varepsilon(|x_{i-\frac{1}{2}} - y|)dy\right) + u_i - u_i^3, \tag{3.7.2}$$

for all $i = 1, 2, \ldots, N$. Using the approximation for u and the midpoint rule for numerical integration, we approximate the first integral in (3.7.1) by

$$\begin{aligned}\sum_{k=1}^N \left(\int_{x_{k-1}}^{x_k} \bar{J}_\varepsilon(|x_{i-\frac{1}{2}} - y|)dy\right) u_k &\approx \sum_{k=1}^N \bar{J}_\varepsilon(|x_{i-\frac{1}{2}} - x_{k-\frac{1}{2}}|)u_k\Delta x \\ &= \sum_{k=1}^N \bar{J}_\varepsilon(x_{|i-k|})u_k\Delta x.\end{aligned}$$

Similarly, the second integral in (3.7.1) is approximated by

$$\sum_{k=1}^N \bar{J}_\varepsilon(x_{|i-k|})\Delta x.$$

Thus, the functions $u_i(t)$ satisfy the ordinary differential equations

$$\frac{du_i}{dt} = \frac{\gamma}{\varepsilon}\left(\sum_{k=1}^N \bar{J}_\varepsilon(x_{|i-k|})u_k - u_i\sum_{k=1}^N \bar{J}_\varepsilon(x_{|i-k|})\right)\Delta x + u_i - u_i^3,$$

for all $i = 1, 2, \ldots, N$. which can be rewritten in the form

$$\frac{d}{dt}U = \frac{\gamma}{\varepsilon}\Gamma U\Delta x - g(U). \tag{3.7.3}$$

Here we have set $U = [u_1\ u_2\ \ldots\ u_N]^T$, $g(U) = [f(u_1)\ f(u_2)\ \ldots\ f(u_N)]^T$, and Γ is a symmetric matrix with elements

$$a_{ik} = \begin{cases} \bar{J}_\epsilon(x_{|i-k|}) & , i \neq k \\ J(0) - \sum_{j=1}^{N} \bar{J}_\epsilon(x_{|i-j|}) & , i = k. \end{cases} \tag{3.7.4}$$

The matrix Γ has real eigenvalues; one is zero and all the other eigenvalues are negative. This system can be solved using standard ODE packages in MATLAB.

3.7.2 Numerical experiments

In this section we present the results of numerical simulations of the equation (3.3.1) using the numerical approximation described above. In the first two experiments of this section we take $N = 140$, $f(u) = u^3 - u$, and

$$J(x) = \begin{cases} 0 & , \quad x = 0 \\ \frac{40}{\sqrt{\pi}} \exp(-400x^2), & x > 0. \end{cases}$$

Experiment 1. We fix $\epsilon = 1$, and take the initial data

$$u_0(x) = 4x(1-x)\sin(10\pi x^2), \quad x \in (0,\, 1). \tag{3.7.5}$$

Time evolutions of the initial data to equilibrium for two values of the parameter γ, namely $\gamma = 0.2$ and $\gamma = 0.39$, are shown in Figures 3.5 and 3.7, respectively. In the first figure we see that the solution through u_0 does not coarsen at all, while in the second one only a partial coarsening can be observed. As shown in Figure 3.7, a pattern of phase domains where $u \approx \pm 1$ and transition layers quickly develop, followed by the shrinkage of the smaller scale domains. The latter process appears to be much slower than the first one. Finally, a steady state solution is attained at time $t \approx 160$, a fact which also can be observed from Figure 3.8, which contains the graph of the Lyapunov function (3.2.8) versus time with $\gamma = 0.39$ and $\varepsilon = 1$.

Experiment 2. We now fix $\gamma = 1$ and let ε to vary. The same initial data is used. As shown in Figure 3.6, if $\epsilon = 0.2$ the solution through u_0 does not coarsen at all. Figure 3.9 illustrates the evolution of the solution having $\varepsilon = 0.35$ through to equilibrium. Again, domains where $u \approx \pm 1$ separated by transition layers quickly appear, followed by the dissappearance of the smaller domains while the bigger ones grow. After the formation of positive and negative domains, the profile is undergoing a slower evolution that in the previous case, a fact which can be also observed in the plot of the Lyapunov functional (3.2.8). The equilibrium solution is partially coarsened and is attained when $t \approx 300$.

In Figures 3.11 and 3.12 we see the initial data $u_0(x)$ and final equilibrium solutions for a range of values of γ and ε, respectively, while the other parameter is fixed to be 1. One can observe some similarities between these stationary solutions. For both $\gamma = 0$ or $\varepsilon \to 0$, the equilibrium solution is $u = \text{signum}(u_0)$. When γ, respectively ε, is big enough, the steady state is either $+1$ or -1, depending on the sign of $u_0(0)$.

Experiment 3. We perform a two dimensional experiment on a unit square. In the approximation we use a 25×25 grid. In this experiment $\epsilon = 1$, $\gamma = 0.8$, $\Delta t = 0.4$, and

$$J(x) = \begin{cases} 0 & , \quad x = 0 \\ \dfrac{100}{\pi} \exp(-25|x|^2), & x \neq 0. \end{cases}$$

The initial data u_0 is taken to be such that its value at each lattice site is a randomly generated number between -1 (black) and 1 (white). As we can see in Figure 3.13 the solution through u_0 partially coarsens to a spatially inhomogeneous equilibrium, also represented in Figure 3.14.

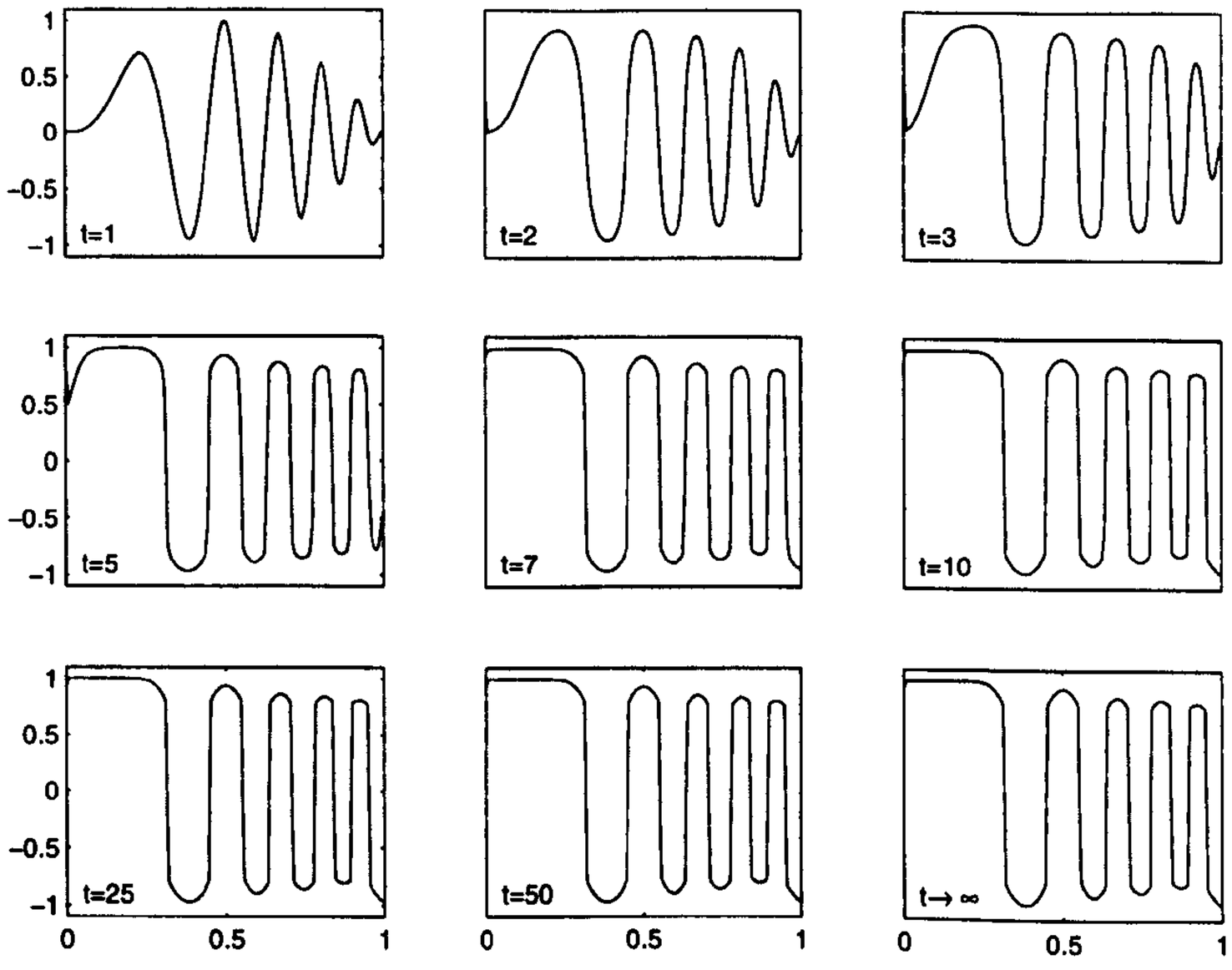

Figure 3.5: Time evolution of the solution of (3.7.1) with $\gamma = 0.2$ and $\varepsilon = 1$.

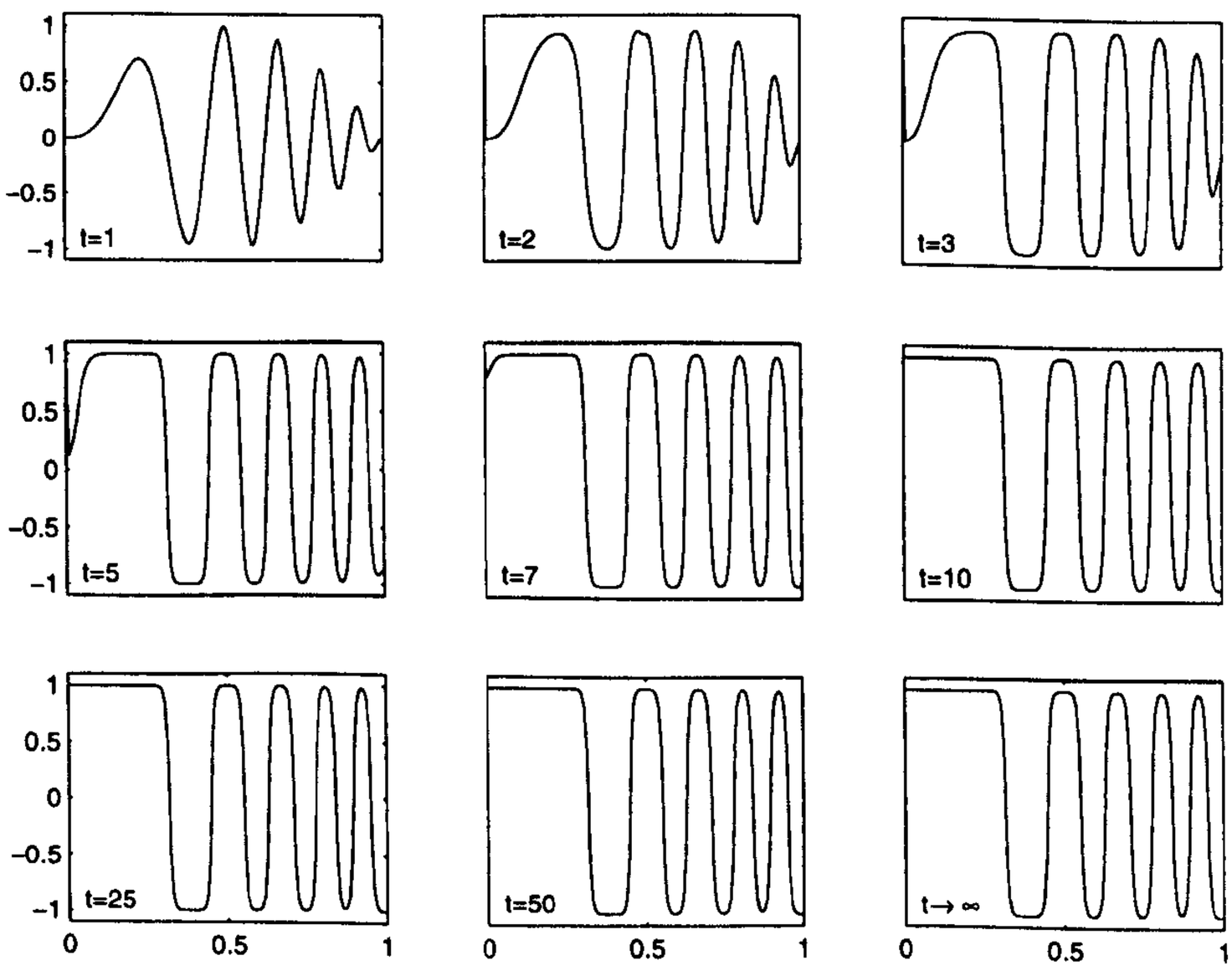

Figure 3.6: The Lyapunov function (3.2.8) against time, for $\epsilon = 0.2$ and $\gamma = 1$.

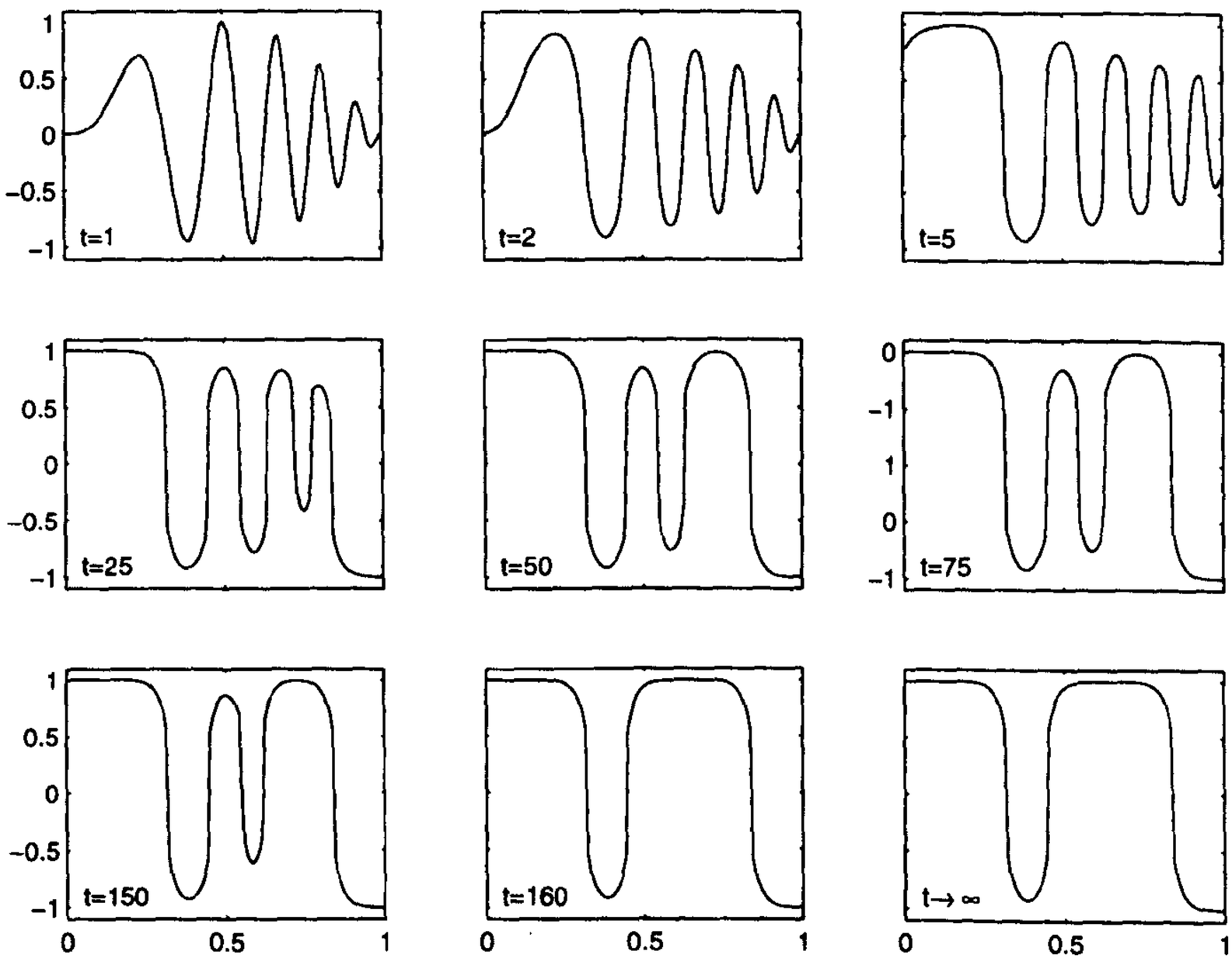

Figure 3.7: Time evolution of the solution of (3.7.1) with $\gamma = 0.39$ and $\varepsilon = 1$.

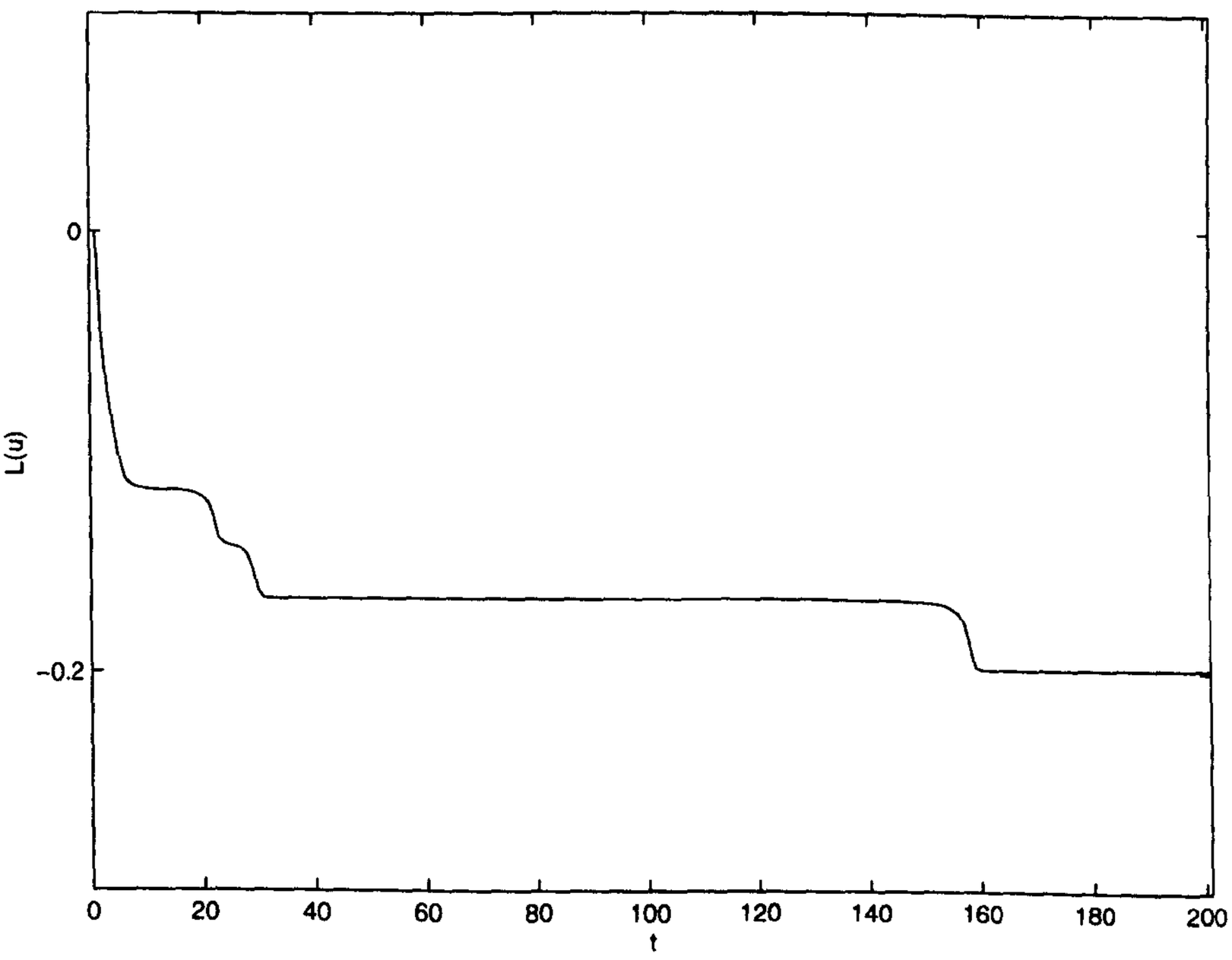

Figure 3.8: The Lyapunov function (3.2.8) against time, for $\gamma = 0.39$ and $\varepsilon = 1$.

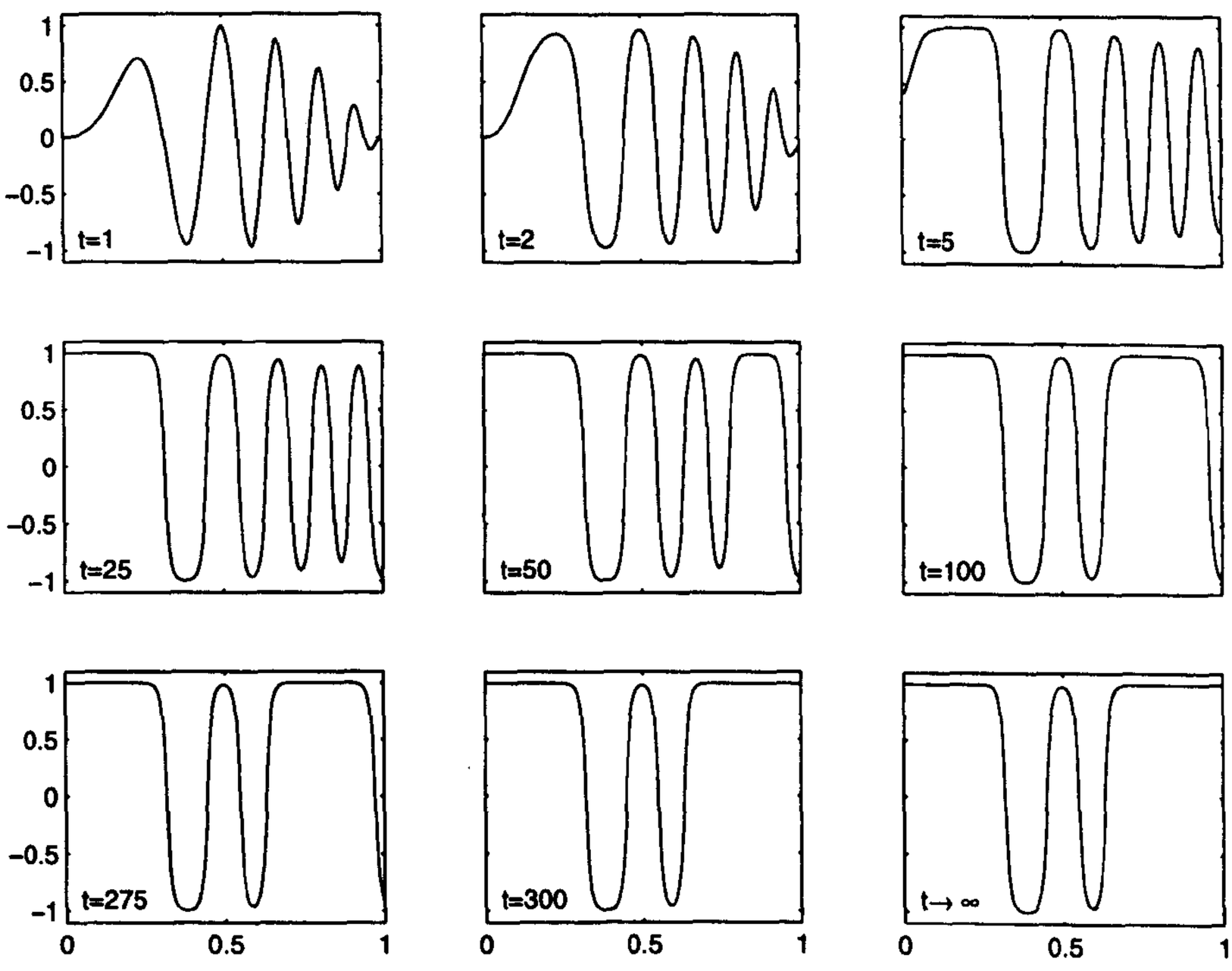

Figure 3.9: Time evolution of the solution of (3.7.1) with $\gamma = 1$ and $\varepsilon = 0.35$.

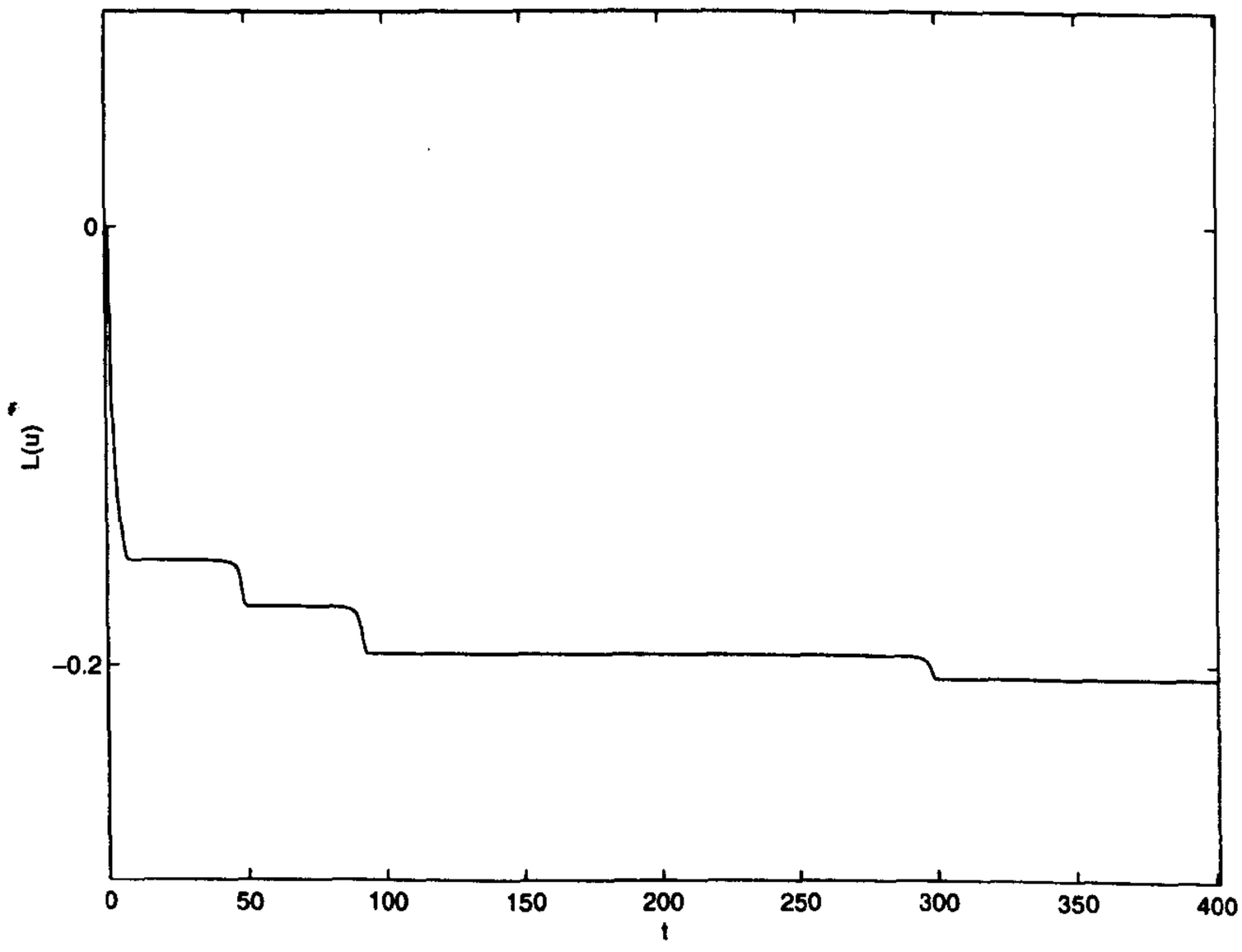

Figure 3.10: The Lyapunov function (3.2.8) against time, for $\gamma = 1$ and $\varepsilon = 0.35$.

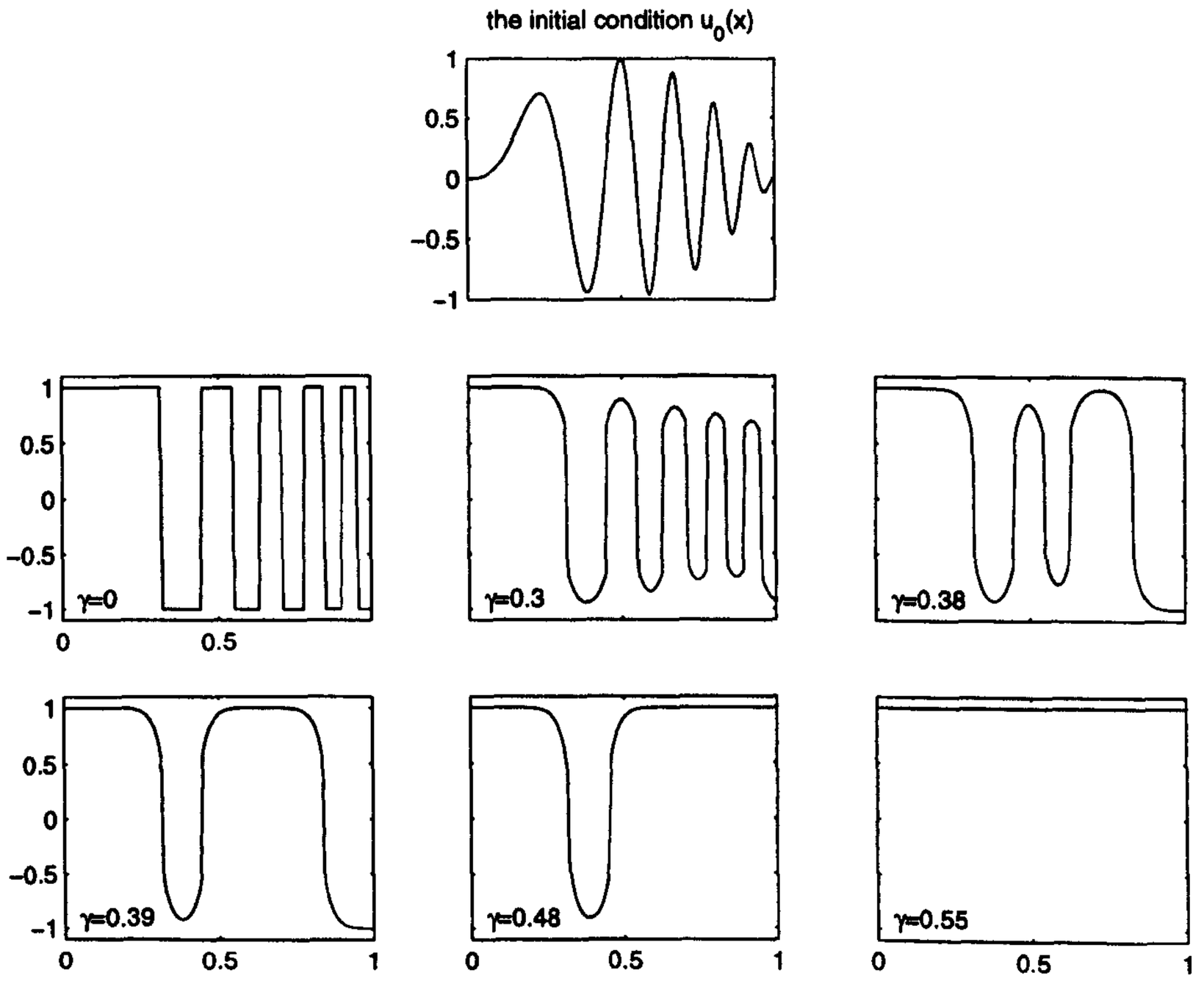

Figure 3.11: Equilibrium solutions of (3.7.1) for different values of γ.

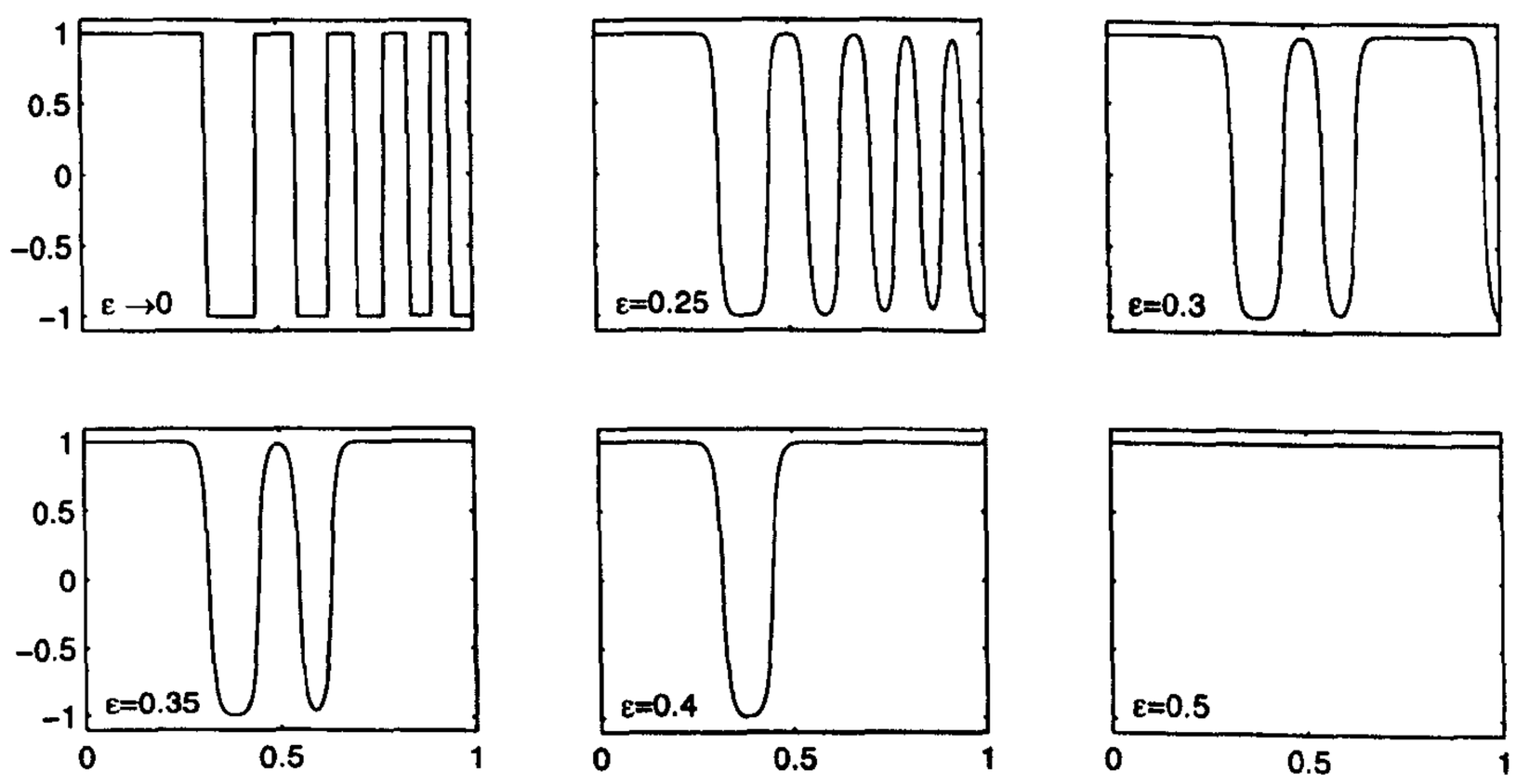

Figure 3.12: Equilibrium solutions of (3.7.1) for different values of ε.

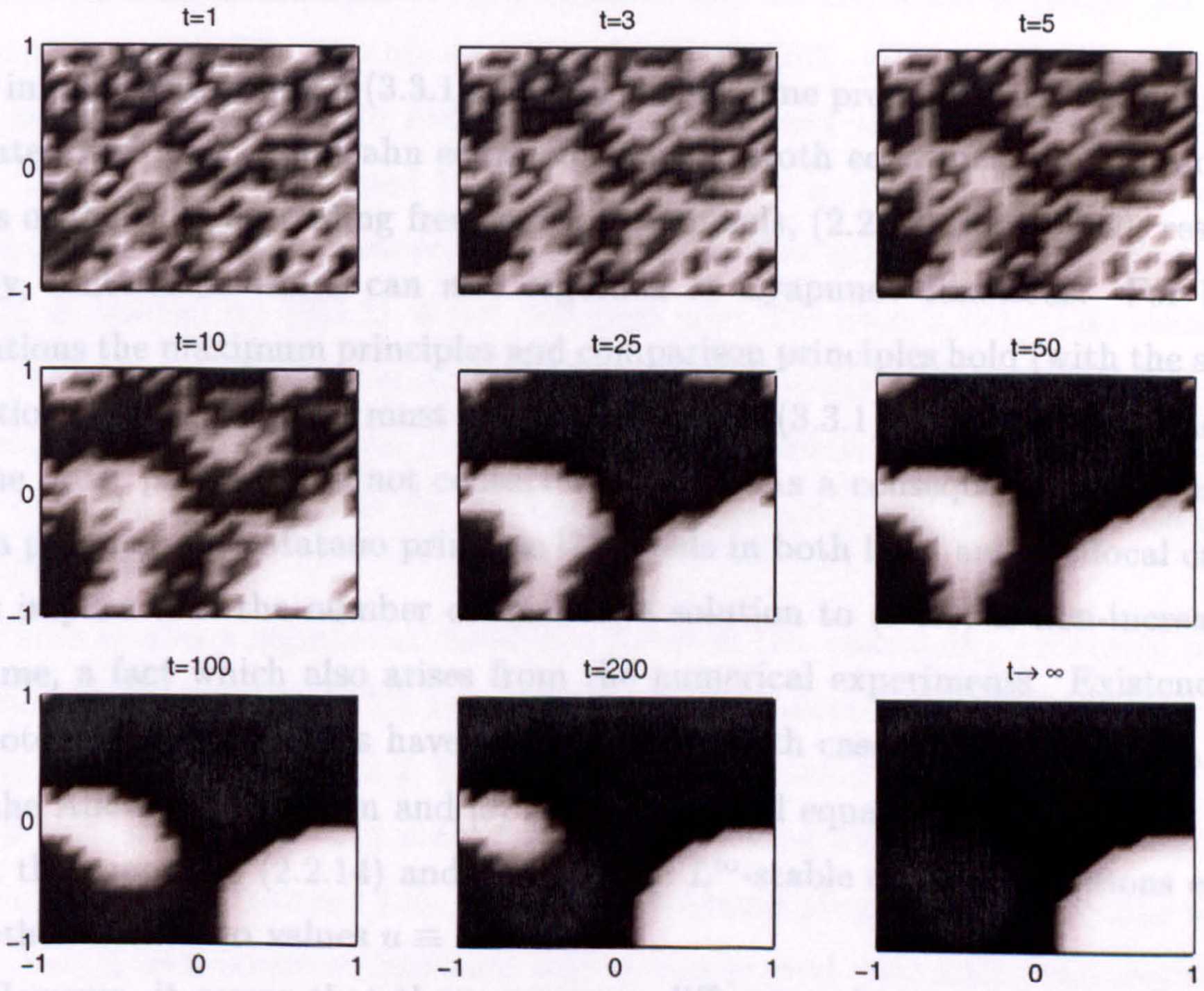

Figure 3.13: Time evolution of a solution of (3.7.1) with $\gamma = 0.8$ in two space dimensions.

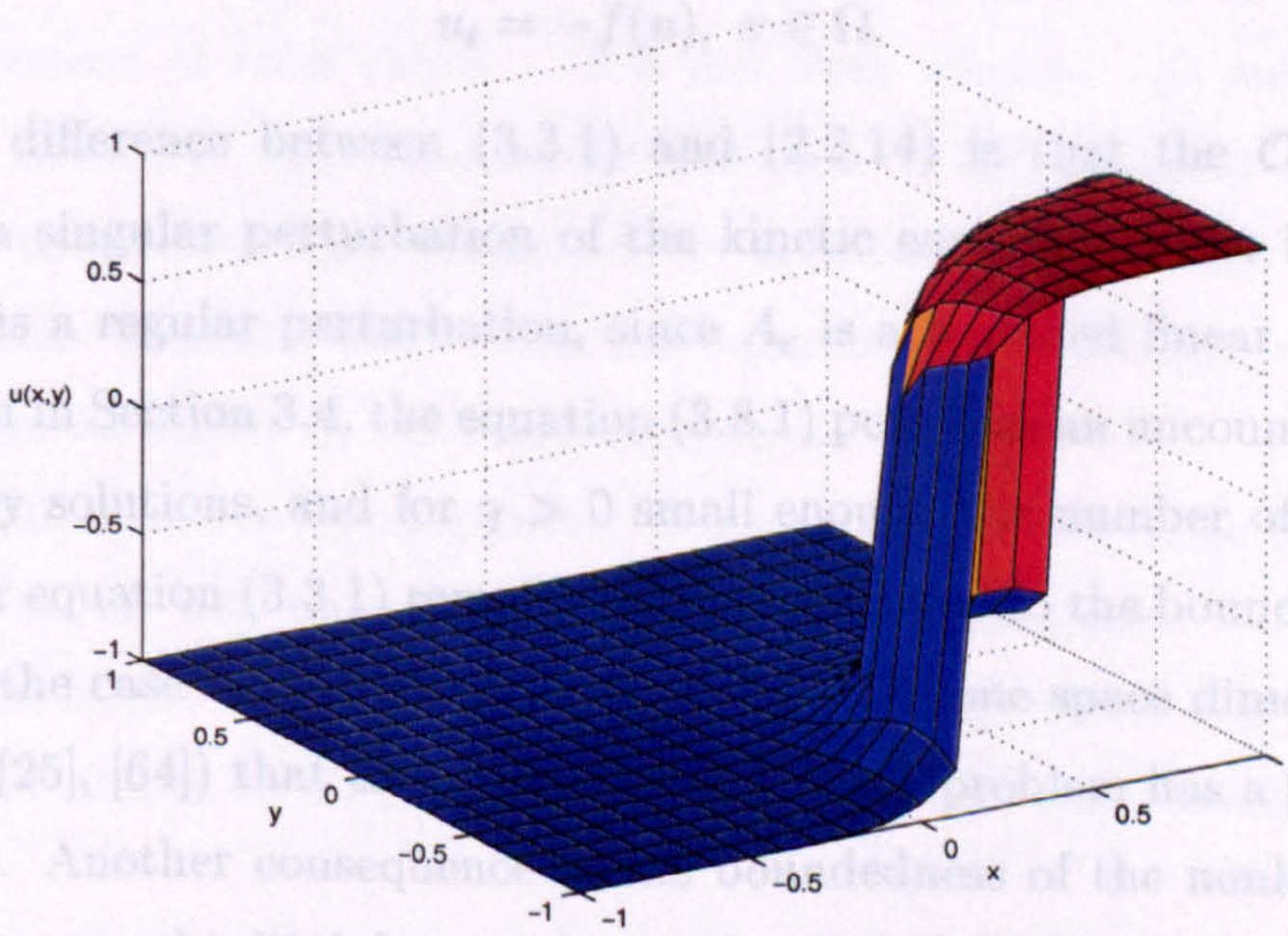

Figure 3.14: Equilibrium solution of (3.7.1) with $\gamma = 0.8$.

3.8 Conclusions

The initial-value problem (3.3.1)+(3.3.5) shares some properties with the one associated with the Allen-Cahn equation (2.2.14). Both equations are L^2-gradient flows of their corresponding free energy functionals, (2.2.12) and (3.3.9), respectively, functionals which can also regarded as Lyapunov functions. For both equations the maximum principles and comparison principles hold (with the specification that the kernel J must be non-negative in (3.3.1)), and the total amount of the order parameter is not conserved in time. As a consequence of the maximum principle, the Matano principle [76] holds in both local and nonlocal cases. This implies that the number of zeros of a solution to (3.3.1) is non-increasing in time, a fact which also arises from the numerical experiments. Existence of monotone travelling waves have been shown in both cases (see for example, [47] for the Alle-Cahn equation and [9] for the nonlocal equation). If $f(u) = u^3 - u$, then the equations (2.2.14) and (3.3.1) have L^∞-stable constant solutions equal to either of the two values $u \equiv \pm 1$.

However, it seems that there are more differences between these evolutions than similarities. If we consider the kinetic equation obtained by setting γ to zero in the integro-differential equation (3.3.4) or the Allen-Cahn equation (2.2.14), we get

$$u_t = -f(u), \ x \in \Omega. \tag{3.8.1}$$

The major difference between (3.3.1) and (2.2.14) is that the $\mathcal{O}(\varepsilon^2)$ term in (2.2.14) is a singular perturbation of the kinetic equation, while in (3.3.4) the $\mathcal{O}(\gamma)$ term is a regular perturbation, since A_ε is a bounded linear operator. As we have seen in Section 3.4, the equation (3.8.1) possesses an uncountable number of stationary solutions, and for $\gamma > 0$ small enough the number of steady state solutions for equation (3.3.1) remains uncountable, due to the boundedness of A_ε. This is not the case for the Allen-Cahn equation; in one space dimension, it was shown (see [25], [64]) that the associated stationary problem has a finite number of solutions. Another consequence of the boundedness of the nonlocal operator is that for a general initial data one can solve (3.3.1) forwards and backwards in time (if f is bounded, for example), but the local equation can only be solved

forward in time. While (2.2.14) is a gradient system and a whole theory for such systems is applicable for this equation (see [62], [63], [64]), the nonlocal equation is not, since it fails to fulfill the precompactness requirement in Definition 2.8. The evolution governed by (2.2.14) possesses a compact attractor formed by equilibria and their connecting orbits, while the attractor of the dynamical sytem generated by (3.3.1) is not compact (see Theorem 3.17). The stabilisation of solutions of the Allen-Cahn equation to a steady state follows easily as a consequence of precompactness of the generated semigroup, and it is not obvious how to prove such a result for the nonlocal equation, even though stabilisation for (3.8.1) is trivial.

There is also a significant difference between the coarsening processes of the solutions to (2.2.14) and (3.3.1) for small enough values of the parameters ε or γ: as explained in Section 2.2.2, for all $\varepsilon > 0$ we have coarsening to one of the two stable solutions in the first case, and non-coarsening for small enough ε or γ in the latter one (see Section 3.5). The non-coarsening property is mainly due to the fact that A_ε is a bounded operator, and it was proved only under the restriction $\|u_0\| < 1$. In the final chapter we discuss how this assumption can be removed.

By expanding the nonlocal term in the expression of the free energy (3.2.3) in Taylor series and truncating the result, we find some unbounded flows which are not always well-posed, the well-posedness depending on the order of truncation and the direction of time chosen. It is not clear whether the solutions to the unbounded flows can approximate the solution to the bounded flow given by (3.3.1). By using Padé approximation, we approximated the flow generated by (3.3.1) by some bounded flows. The new equations have the advantage of being well-posed for all orders of the Padé approximation.

In equation (2.2.14) the parameter ε can represent the range of interactions in the system, as well as the strength of those interactions. For the nonlocal equation this fact is not possible, and this justifies the use of two dimensionless parameters, ε and γ, to represent the above quantities, respectively.

Chapter 4

Nonlocal mass-conserving equations

4.1 Introduction

As one can easily observe, the nonlocal Allen-Cahn equation discussed in the previous chapter does not conserve the average value of the order parameter, which is not an issue if we are modelling phase transitions in ferromagnetic materials. If instead we are modelling phase change in binary alloys, then the total amount of each species in the system must be conserved and consequently, the evolutionary equation that models the phenomenon must have this property. This chapter deals with two mass-conserving integro-differential equations, more precisely with two nonlocal versions of the equations (2.2.20) and (2.2.19), which we propose as alternative models for the phase separation in binary alloys. The consideration of these equations is motivated by the discussion in [66], which concluded that the Cahn-Hilliard model fails to be applied when the scale of microstructure is very small. As we pointed out in Section 2.2.1, one can avoid the gradient expansion of the free energy by considering instead the functional (2.2.13).

A natural way to derive an equation for the time evolution of a system is to consider constrained gradient flows of the free energy functional (3.2.3) on an

appropriate linear manifold $\mathcal{M}$, in an appropriate Hilbert space H. If the system is confined to a bounded region Ω, and we choose $H = L^2(\Omega)$ and $\mathcal{M}$ to be the set of $L^2(\Omega)$ functions having the same mass, then the constrained gradient flow in the sense of the $L^2(\Omega)$ inner product leads to a nonlocal equation similar to the nonlocal reaction-diffusion equation (2.2.20), which instead of the Laplacian contains a bounded nonlocal operator.

However, different choices of the Hilbert space, as well as of the inner product, will produce different evolutionary equations. As we shall see later in this chapter, by choosing a suitable inner product in the space of the $L^2(\Omega)$ functions having zero-mass we get a similar equation to the Cahn-Hilliard equation in which, once again, the Laplacian is replaced by a bounded nonlocal operator. These two new equations can be used as alternatives for their local analogues, and some of their properties are studied in the following sections of this chapter.

We start this chapter by deriving these equations. Then we discuss some properties of their time-independent solutions, followed by a linear analysis and a discussion on the dispersion relation. At the end of the chapter we outline some numerical experiments for both models, showing that the non-coarsening phenomenon observed and proved in the last chapter for the nonlocal Allen-Cahn equation is also common for these equations.

4.2 A nonlocal mass-conserving version of the reaction-diffusion equation

This section deals with the following mass-conserving nonlocal equivalent of the reaction-diffusion equation

$$u_t = \frac{\gamma}{\varepsilon}\int_\Omega J(\frac{|x-y|}{\varepsilon})(u(y)-u(x))\,dy - f(u) + \frac{1}{|\Omega|}\int_\Omega f(u(y))dy, \quad x \in \Omega,\ t>0, \tag{4.2.1}$$

where $\Omega \subset \mathbb{R}$ is a convex bounded domain, $|\Omega|$ is the Lebesque measure of Ω, and J, f, γ and ε are as in the introduction of Chapter 3. Moreover, we shall assume throughout this chapter that $J(\cdot) > 0$ on Ω.

4.2.1 Derivation of the equation

In order to get (4.2.1), we firstly derive the mass-conserving gradient flow of the free energy (3.2.3) with respect to the $L^2(\mathbb{R})$ inner product, and then we restrict the equation to Ω. We use the notations $< \cdot, \cdot >$ and $\| \cdot \|$ for the inner product and, respectively, for the norm in L^2. Let us consider the linear subspace of $L^2(\mathbb{R})$ of functions with average (mass) zero,

$$\mathcal{M}_0 = \{u \in L^2(\mathbb{R}), \int_{\mathbb{R}} u(x)dx = 0\},$$

and for a given $\overline{u} \in L^2(\mathbb{R})$ we introduce the affine linear manifold

$$\mathcal{M} = \overline{u} + \mathcal{M}_0.$$

Due to the constraint (2.2.6), our interest is now to find the constrained gradient $\text{grad}_{\mathcal{M}} E_K(u)$ which, by Definition 2.11, must be an element of $\overline{\mathcal{M}_0} = \mathcal{M}_0$. Using (3.2.4), for all $v \in \mathcal{M}_0$ and $C \in \mathbb{R}$ we have

$$\begin{aligned} < \text{grad}_{\mathcal{M}} E_K(u), v > &= < \gamma \int_{\mathbb{R}} J(|x-y|)[u(x)-u(y)]dy + f(u), v > \\ &= < \gamma \int_{\mathbb{R}} J(|x-y|)[u(x)-u(y)]dy + f(u) + C, v >, \end{aligned}$$

implying that

$$-\gamma \int_{\mathbb{R}} J(|x-y|)[u(y)-u(x)]dy + f(u) - C$$

is a candidate for the gradient. Since the gradient must be in $\mathcal{M}_0$, we get

$$C = \int_{\mathbb{R}} f(u(y))\, dy.$$

We thus obtain the gradient in $\mathcal{M}$,

$$\text{grad}_{\mathcal{M}} E_K(u) = -\gamma \int_{\mathbb{R}} J(|x-y|)[u(y)-u(x)]dy + f(u) - \int_{\mathbb{R}} f(u(y))\, dy,$$

and the corresponding evolution equation

$$u_t = \gamma \int_{\mathbb{R}} J(|x-y|)[u(y)-u(x)]dy - f(u) + \int_{\mathbb{R}} f(u(y))\, dy, \;\; x \in \mathbb{R}, \;\; t > 0.$$

Rescaling the space by a positive constant ε and then restricting the problem to Ω yields (4.2.1). As we can readily check, we have

$$\frac{d}{dt} \int_{\Omega} u(x)\, dx = 0, \tag{4.2.2}$$

which means that the mass is preserved for the evolution governed by (4.2.1), as required.

4.2.2 The semigroup approach

We consider the following initial-value problem in a convex bounded domain $\Omega \subset \mathbb{R}$:

$$(NRS) \quad \begin{cases} u_t = \gamma \displaystyle\int_\Omega J_\varepsilon(|x-y|)[u(y)-u(x)]dy - f(u) + \frac{1}{|\Omega|}\int_\Omega f(u(y))\,dy \\ u(0) = u_0, \end{cases}$$

where J_ε is the given by (3.3.2). Because this equation conserves mass, spaces with an integral constraint are appropriate to work with. We suppose that the average of u over Ω is M, that is (2.2.6) is satisfied, and denote by X the Hilbert space

$$X = \{u \in L^2(\Omega);\ \frac{1}{|\Omega|}\int_\Omega u(y)\,dy = 0\}, \tag{4.2.3}$$

endowed with the norm induced by the L^2-norm. In order to work in this space we perform a change of variable and set $\hat{u} = u - M$. We obtain

$$\hat{u}_t = \gamma \int_\Omega J_\varepsilon(|x-y|)[\hat{u}(y)-\hat{u}(x)]dy - f(\hat{u}+M) + \frac{1}{|\Omega|}\int_\Omega f(\hat{u}(y)+M)\,dy, \quad t>0.$$

Dropping the caret from $\hat{u}$ we have the evolution equation

$$u_t = \gamma A_\varepsilon u - f(u+M) + \frac{1}{|\Omega|}\int_\Omega f(u(y)+M)\,dy, \quad t>0, \tag{4.2.4}$$

where A_ε is the operator given by (3.3.3). We would like to prove that the family of solutions to (4.2.4) with $u(0) = u_0$ forms a continuous semigroup on X. We rewrite the initial-value problem in the form

$$(P) \begin{cases} u_t = \gamma A_\varepsilon u + g(u), \quad t>0, \\ u(0) = u_0, \end{cases}$$

where

$$g(u) = -f(u+M) + \frac{1}{|\Omega|}\int_\Omega f(u(y)+M)\,dy, \quad x \in \Omega.$$

We start with the following lemma:

Lemma 4.1 *The linear operator A_ε given by (3.3.3) is bounded, non-positive and self-adjoint on X.*

Proof. Obviously, $A_\varepsilon u \in X$. For all $u \in X$ we have

$$\begin{aligned} < A_\varepsilon u,\, u > &= \int_\Omega \int_\Omega J_\epsilon(|x-y|)u(x)[u(y)-u(x)]dydx \\ &= -\frac{1}{2}\int_\Omega \int_\Omega J_\epsilon(|x-y|)[u(y)-u(x)]^2 dydx \\ &\leq 0, \end{aligned} \tag{4.2.5}$$

and thus A_ε is non-positive. The boundedness follows from (4.2.5) and the following argument. For all $u \in X$,

$$\begin{aligned} < A_\varepsilon u,\, u > &\geq -\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u^2(y)+u^2(x)]dydx \\ &= -2\int_\Omega \int_\Omega J_\epsilon(|x-y|)u^2(x)dydx \\ &= -2\int_\Omega \left(\int_\Omega J_\varepsilon(|x-y|)\,dy\right) u^2(x)dx \\ &\geq -2\int_\Omega \left(\int_{\mathbb{R}} J_\varepsilon(|x-y|)\,dy\right) u^2(x)dx \\ &= -2\left(\int_{\mathbb{R}} J_\epsilon(|\eta|)d\eta\right)\|u\|^2 \\ &= -2\,\|u\|^2. \end{aligned}$$

For all $u,\ v \in X$, we have

$$\begin{aligned} < A_\varepsilon u,\, v > &= \int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u(y)-u(x)]v(x)\,dydx \\ &= -\frac{1}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u(y)-u(x)][v(y)-v(x)]\,dydx \\ &= \int_\Omega \int_\Omega J_\epsilon(|x-y|)u(x)[v(y)-v(x)]\,dydx \\ &= < u,\, A_\varepsilon v >, \end{aligned}$$

which shows that A_ε is self-adjoint. □

Lemma 4.2 *If $f : L^2(\Omega) \to L^2(\Omega)$ is locally Lipschitz, then the operator $g : X \to X$ is locally Lipschitz.*

Proof. Obviously $g(u) \in X$. For any $c > 0$ and $u, v \in X$ with $\|u\| \leq c$, $\|v\| \leq c$, we have

$$\begin{aligned}
&\int_\Omega [g(u)(x) - g(v)(x)]^2\, dx = \\
&\quad = \int_\Omega \Big[f(u(x) + M) - f(v(x) + M) - \\
&\qquad\qquad -\frac{1}{|\Omega|}\int_\Omega (f(u(y) + M) - f(v(y) + M))\, dy \Big]^2 dx \\
&\leq\ 2\int_\Omega [f(u(x) + M) - f(v(x) + M)]^2\, dx + \\
&\qquad\qquad +\frac{2}{|\Omega|^2}\int_\Omega \Big[\int_\Omega |f(u(y) + M) - f(v(y) + M)|\, dy\Big]^2 dx \qquad (4.2.6) \\
&\leq 2\|f(u(x) + M) - f(v(x) + M)\|^2 + 2\int_\Omega [f(u(y) + M) - f(v(y) + M)]^2\, dy \\
&=\ 2\|f(u + M) - f(v + M)\|^2 + 2\|f(u + M) - f(v + M)\|^2 \\
&\leq\ 4L_c^2\|u - v\|^2,
\end{aligned}$$

which implies that $g : X \to X$ is locally Lipschitz, with Lipschitz constant $2L_c$.

Note that inequality (4.2.6) has been obtained using the inequality $(a - b)^2 \leq 2a^2 + 2b^2$, and the second integral in (4.2.6) was evaluated using the Cauchy-Schwarz formula. □

We define a *solution* for the problem (P) on an interval $[0, T)$ to be a continuous function $u : [0, T) \to X$, such that $g(u(\cdot)) : [0, T) \to X$ is continuous, u satisfies $(P)_1$ on $(0, T)$ and $u(0) = u_0$. We have the following existence and uniqueness result:

Theorem 4.3 *Suppose J satisfies the conditions $(\mathcal{H}_1)$, f is locally Lipschitz on $L^2(\Omega)$ and satisfies (3.6.26). Then for any initial data $u_0 \in X$ the problem (P) has a unique global solution $u(t, x; u_0)$ such that $u \in C^1([0, \infty), X)$. For all $T > 0$ the mapping $u_0 \mapsto u$ is Lipschitz continuous from X into $C([0, T), X)$.*

Proof. The local existence and uniqueness of a solution defined on a maximal domain $[0, T_{u_0})$ follows from the theory of locally Lipschitz perturbations of bounded operators on Banach spaces (See, for example, [64] Theorem 3.3.3.).

We now prove that the solution is defined for any $t > 0$. We consider the functional (3.3.9). For all solutions $u(t) \in X$ we have

$$\frac{d}{dt}\mathcal{L}(u) = -\int_\Omega u_t^2\,dx \le 0. \tag{4.2.7}$$

Furthermore, for any $\mu > 0$, condition (3.6.26) implies that there is a positive constant C_μ such that

$$\begin{aligned} F(s) &= \int_0^u [\frac{f(r)}{r} - 2\mu]r\,ds + \mu s^2 \\ &\ge -C_\mu + \mu s^2, \quad \text{for } s > 0. \end{aligned}$$

For $s < 0$, one can obtain a similar estimate for $F(s)$ so that

$$F(s) \ge \mu s^2 - C_\mu, \quad \text{for all } s \in \mathbb{R}. \tag{4.2.8}$$

For any $u \in X$, relations (4.2.7) and (4.2.8) imply

$$\mu\|u\|^2 - C_\mu \le \mathcal{L}(u) \le \mathcal{L}(u_0) \le C,$$

from which we get the boundedness of u in the norm of X, and thus the solution is globally defined. We now prove the continuous dependence of the solution on the initial data. For all $T > 0$ we take any two solutions of (P) on $[0, T)$, $u(t)$, $v(t) \in X$, and write

$$(u-v)_t = \gamma A_\varepsilon(u-v) - (f(u)-f(v)) + \frac{1}{|\Omega|}\int_\Omega [f(u(y))-f(v(y))]\,dy, \text{ for } 0 \le t < T.$$

Taking the L^2-inner product of this equation with $u - v$ (which has zero-mass) and using the non-positiveness of A_ε and the locally Lipschitz property of f, we obtain

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|u-v\|^2 &\le - < f(u) - f(v),\, u - v > \\ &\le L\|u-v\|^2, \end{aligned}$$

with $L > 0$, which gives

$$\|u(t) - v(t)\|^2 \le e^{2LT}\|u_0 - v_0\|^2.$$

This completes the proof. □

Remark 4.4 The family of solution operators, $\{T(t) : X \to X,\ t \geq 0\}$, given by $T(t)u_0 = u(x,\, t;\, u_0)$, defines a continuous semigroup on X. It can be shown that the fuctional $\mathcal{L}(u)$ is a Lyapunov function for the semigroup.

Remark 4.5 In the particular case $f(u) = \alpha_2 u^3 + \alpha_1 u^2 - u$, the hypothesis (3.6.26) is equivalent to the condition $\alpha_2 > 0$. Following the discussion in [39] regarding solutions of the Cahn-Hilliard equation, where it was proved that the sign of α_2 is crucial for the existence of a global solution, we can show that this is also the case here. If $\alpha_2 < 0$ (that is, (3.6.26) is not satisfied), then solutions starting from initial data with low energy will blow up in finite time. Indeed, we have the following theorem:

Theorem 4.6 *If $\alpha_2 < 0$ and $\mathcal{L}(u_0)$ is sufficiently low, then there is a time $T^* > 0$ such that*

$$\lim_{t \to T^*} \|u(t)\|_2 = \infty. \tag{4.2.9}$$

Proof. The Lyapunov function $\mathcal{L}(u)$ can be written in the form

$$\mathcal{L}(u) = \frac{\gamma}{2} < -A_\epsilon u,\, u > + \int_\Omega F(u(x))\, dx. \tag{4.2.10}$$

Since $\mathcal{L}(u(t))$ is decreasing in time, we get

$$\gamma < -A_\epsilon u,\, u > \leq\ 2\mathcal{L}(u_0) - 2\int_\Omega F(u(x)\, dx.$$

Let us take the L^2-scalar product of (4.2.4) with $u \in X$. Using the previous inequality, we obtain

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|u(t)\|^2 &= -\gamma < -A_\epsilon u,\, u > - < f(u+M),\, u > \\
&\geq 2\int_\Omega F(u(x))\, dx - < f(u+M),\, u > -2\mathcal{L}(u_0) \\
&= -\frac{\alpha_2}{4}\int_\Omega u^4(x)\, dx - \zeta_1 \int_\Omega u^3(x)\, dx - \zeta_2 \int_\Omega u^2(x)\, dx - \\
&\quad -\frac{\alpha_2}{4}\int_\Omega u^4(x)\, dx - 2\mathcal{L}(u_0),
\end{aligned} \tag{4.2.11}$$

where

$$\zeta_1 = 3\alpha_2 M + \frac{\alpha_1}{3} \quad \text{and} \quad \zeta_2 = (3\alpha_2 M + 2\alpha_1)M.$$

Since $\alpha_2 < 0$, there is a positive constant C (depending on α_1, α_2 and Ω) such that

$$-\frac{\alpha_2}{4}\int_\Omega u^4(x)\,dx - \zeta_1\int_\Omega u^3(x)\,dx - \zeta_2\int_\Omega u^2(x)\,dx + C \geq 0.$$

The Cauchy-Schwarz inequality implies that

$$\left(\int_\Omega u^2(x)\,dx\right)^2 \leq |\Omega|\int_\Omega u^4(x)\,dx.$$

Combining the last two inequalities with (4.2.11), gives

$$\frac{d}{dt}\|u(t)\|^2 \geq C_1\|u(t)\|^4 - 2C - 4\mathcal{L}(u_0),$$

with $C_1 = -\dfrac{\alpha_2}{2|\Omega|} > 0$. If initial data is such that

$$\mathcal{L}(u_0) < -\frac{C}{2},$$

then the limit (4.2.9) holds. □

Remark 4.7 By exhibiting positively invariant regions for u, one can also show the global existence of a solution $u(t) \in L^\infty(\Omega)$. We can prove the following result:

Proposition 4.8 *Let $[a, b]$ be any interval on which f satisfies the condition*

$$f(a) < f(u) < f(b), \quad \textit{for all } u \in (a, b).$$

If $u(x, t)$ is a solution to $(P)_1$ in $\Omega \times [0, T]$ and $u_0(x)$ is contained in (a, b), for all $x \in \Omega$, then $u(x, t) \in (a, b)$, for all $(x, t) \in \Omega \times [0, T]$.

Proof. Let us suppose, by contradiction, that there exists a first time t_0, $0 < t_0 \leq T$, such that $u(x, t)$ leaves the interval (a, b), i.e., for some $x_0 \in \Omega$ we have $u(x_0, t_0) = a$ or b. We take $u(x_0, t_0) = b$, the other case being similar. It follows that

$$u_t(x_0, t_0) \geq 0,$$

and

$$\begin{aligned} A_\varepsilon u(x_0, t_0) &= \int_\Omega J_\varepsilon(|x - y|)[u(y, t_0) - u(x_0, t_0)]\,dy \\ &\leq 0. \end{aligned}$$

Using these inequalities in $(P)_1$ we obtain

$$\int_\Omega [f(u(y, t_0)) - f(b)]\, dy \geq 0.$$

Since $a \leq u(y, t_0) \leq b$ for all $y \in \Omega$, the hypothesis on f implies

$$\int_\Omega [f(u(y, t_0)) - f(b)]\, dy \leq 0,$$

and thus we can only have $f(u(y, t_0)) = f(b)$, for all $y \in \Omega$, which means that $u(y, t_0) \equiv b$. But this contradicts the mass constraint (2.2.6). A similar argument in the case $u(x_0, t_0) = a$ proves the lemma. □

Corollary 4.9 (global existence in $L^\infty(\Omega)$) *Suppose that J satisfies $(\mathcal{H}_1)$, f is locally Lipschitz and satisfies*

$$\liminf_{z\to-\infty} f(z) < f(u) < \limsup_{z\to\infty} f(z), \quad \textit{for all } u \in \mathbb{R}.$$

Then if $u_0 \in L^\infty(\Omega)$, there exists a unique global solution $u(x, t)$ to (P) such that $u \in C^1([0, \infty), L^\infty(\Omega))$.

Proof. The existence and uniqueness of a local solution can be proved by a standard fixed point argument. Then the local solution can be extended to a global one using the above proposition. □

Remark 4.10 Because of the nonlocal term $\int_\Omega f(u)dx$, the comparison principle stated in Lemma 3.5 is no longer valid for solutions of (P).

4.3 The nonlocal Cahn-Hilliard equation

In this section we are concerned with the semigroup approach for a nonlocal version of the Cahn-Hilliard equation (2.2.19), i.e., with the equation

$$u_t = -A_\varepsilon(\gamma A_\varepsilon u - f(u)), \quad x \in \Omega, \ t > 0, \tag{4.3.1}$$

where A_ε is the operator given by (3.3.3).

4.3.1 Derivation of the equation

To derive this equation we shall work in the same Hilbert space X defined in (4.2.3), but endowed with a new inner product. The Fredholm alternative applied to operator $A_\varepsilon : X \to X$ says that for a suitable Ω, and for any function $u \in X$, there is a unique solution $w = \mathcal{S}_\varepsilon(u)$ to the problem

$$\begin{aligned} -A_\varepsilon w &= u \\ \int_\Omega w(x)dx &= 0. \end{aligned} \tag{4.3.2}$$

This is due to the fact that the homogeneous problem has only the trivial solution $w \equiv 0$. Indeed, if w is a solution of the problem

$$\begin{aligned} -A_\varepsilon w &= 0 \\ \int_\Omega w(x)dx &= 0, \end{aligned} \tag{4.3.3}$$

then

$$< -A_\varepsilon w,\, w >:= \frac{1}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[w(x)-w(y)]^2\,dydx = 0,$$

which together with the mass constraint on w and $J_\varepsilon(\cdot) > 0$ on Ω, give $w \equiv 0$.

Let us consider the following product: given $u_1, u_2 \in X$, let

$$\ll u_1, u_2 \gg = < \mathcal{S}_\varepsilon(u_1),\, u_2 > \quad (\equiv < w_1,\, -A_\varepsilon w_2 >), \tag{4.3.4}$$

where $< \cdot, \cdot >$ denotes the L^2-inner product, and $w_i = \mathcal{S}_\varepsilon(u_i)$, $(i = 1, 2)$ are defined by (4.3.2). Since

$$\begin{aligned} < -A_\varepsilon w_1,\, w_2 > &= < w_1,\, -A_\varepsilon w_2 > \\ &= \frac{1}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[w_1(x)-w_1(y)][w_2(x)-w_2(y)]dydx, \end{aligned} \tag{4.3.5}$$

for all $w_1, w_2 \in X$, then

$$< u_1,\, \mathcal{S}_\varepsilon(u_2) > = < \mathcal{S}_\varepsilon(u_1),\, u_2 >, \tag{4.3.6}$$

for all $u_1,\, u_2 \in X$, and so it is clear that (4.3.4) defines an inner product on X, with the induced norm on X given by

$$\begin{aligned} \|\!|u|\!\|^2 &= < \mathcal{S}_\varepsilon(u),\, u > \\ &(\equiv < -A_\varepsilon w,\, w > = \frac{1}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[w(x)-w(y)]^2\,dydx), \end{aligned} \tag{4.3.7}$$

where $w = \mathcal{S}_\epsilon(u)$ is the unique solution of (4.3.2).

Let us find the constrained gradient flow of the free energy $\mathcal{L}(u)$ corresponding to this inner product. We use again Definition 2.11, with $\mathcal{M}_0 = X$ and $\mathcal{M}$ as in Section 4.2.1. Firstly, let us denote by N_ϵ^γ the following operator:

$$N_\epsilon^\gamma u = \gamma A_\epsilon u - f(u). \tag{4.3.8}$$

Following the same steps as in (3.2.4), we obtain

$$\frac{d}{dh}\mathcal{L}(u+hv)|_{h=0} =< \gamma \int_\Omega J_\epsilon(|x-y|)[u(x)-u(y)]dy + f(u), v > .$$

Using (4.3.4), we have:

$$\begin{aligned}\frac{d}{dh}\mathcal{L}(u+hv)|_{h=0} &= < -N_\epsilon^\gamma u, v > \\ &= < \mathcal{S}_\epsilon(A_\epsilon(N_\epsilon^\gamma u)), v > \\ &= \ll A_\epsilon(N_\epsilon^\gamma u), v \gg,\end{aligned}$$

for all $v \in \mathcal{M}_0$. Since

$$\int_\Omega A_\epsilon N_\epsilon^\gamma u(x)\, dx = 0,$$

the gradient of $\mathcal{L}(u)$ in $\mathcal{M}$ corresponding to the inner product $\ll \cdot, \cdot \gg$ is the element of $\overline{\mathcal{M}_0} = X$ given by

$$\text{grad}_{\mathcal{M}}\mathcal{L}(u) = A_\epsilon(\gamma A_\epsilon u - f(u)), \tag{4.3.9}$$

which yields the gradient flow (4.3.1). We can easily check that (4.2.2) is satisfied, and thus (4.3.1) conserves mass.

4.3.2 The semigroup approach

We aim to prove the existence and uniqueness of a solution to the problem

$$(NCH)\quad \begin{cases} u_t = -A_\epsilon(\gamma A_\epsilon u - f(u)), \quad t > 0, \\ \\ u(0) = u_0, \end{cases}$$

in the space X defined by (4.2.3). If we suppose that the average of u over Ω is M, then to be able to work in X we perform a change of variable, as we did in Section 4.2.1. Setting $\hat{u} = u - M$, we obtain

$$\hat{u}_t = -A_\epsilon(\gamma A_\epsilon \hat{u} - f(\hat{u} + M)), \quad t > 0,$$

which after dropping the caret gives

$$u_t = \gamma \mathcal{A}_\varepsilon u + h_\varepsilon(u), \quad t > 0, \tag{4.3.10}$$

where

$$\mathcal{A}_\varepsilon u = -A_\varepsilon(A_\varepsilon u)$$

and

$$h_\varepsilon(u) = A_\varepsilon(f(u+M)). \tag{4.3.11}$$

Lemma 4.11 *The linear operator $\mathcal{A}_\varepsilon : X \to X$ is bounded, non-positive and self-adjoint with respect to the L^2-scalar product.*

Proof. Obviously, $\mathcal{A}_\varepsilon u$ is an element of X since

$$\int_\Omega \mathcal{A}_\varepsilon u(x)\, dx = 0, \quad \text{for all } u \in X.$$

For all $u,\ v \in X$ we have

$$\begin{aligned} < \mathcal{A}_\varepsilon u,\, v > &= < -A_\varepsilon(A_\varepsilon u),\, v > \\ &= - < A_\varepsilon u,\, A_\varepsilon v > \\ &= < u,\, -A_\varepsilon(A_\varepsilon v) > = < u,\, \mathcal{A}_\varepsilon v > \end{aligned}$$

which proves the self-adjointness of $\mathcal{A}_\varepsilon$. Finally, the non-positiveness follows from the above relations by taking $v = u$. We get

$$< \mathcal{A}_\varepsilon u,\, u > = \ -\|A_\varepsilon u\|^2.$$

□

Lemma 4.12 *If f is locally Lipschitz on $L^2(\Omega)$, then the operator $h_\varepsilon : X \to X$ given by (4.3.11) is locally Lipschitz.*

Proof. Obviously, if $u \in X$ then $h_\varepsilon u \in X$. The lemma follows from the following argument: for all $u,\ v \in X$,

$$\begin{aligned} \|h_\varepsilon(u) - h_\varepsilon(v)\| &= \|A_\varepsilon(f(u+M) - f(v+M)\| \\ &\le 2\|f(u+M) - f(v+M)\|. \end{aligned}$$

□

Based on these two lemmas we can prove the theorem which gives the global existence and uniqueness of solutions to (4.3.10) starting from $u(0) = u_0$.

Theorem 4.13 *Assume J satisfies $(\mathcal{H}_1)$, f is locally Lipschitz on $L^2(\Omega)$ and satisfies (3.6.26). Then for any initial data $u_0 \in X$ there exists a unique global solution $u = u(t, x;\ u_0)$ of (NCH) such that $u \in C^1([0, \infty);\ X)$. The mapping $u_0 \mapsto u(t)$ is continuous in X, for all $t > 0$.*

Proof. Taking into account the previous two lemmas, the application of Theorem 3.3.3, [64] provides the local existence and uniqueness of a solution $u = u(t, x,\ u_0)$ defined on a maximal domain $[0, T)$. The extension of this solution to a global one is proved using energy estimation arguments. Considering the free energy (3.3.9), we observe that this is non-increasing since

$$\begin{aligned}\frac{d}{dt}\mathcal{L}(u) &= \ll \operatorname{grad}_{\mathcal{M}}\mathcal{L}(u),\ u_t \gg \\ &= \ll A_\varepsilon(N_\varepsilon^\gamma u),\ u_t \gg \\ &= \ll -u_t,\ u_t \gg \\ &= -\|\|u_t\|\|^2, \quad \text{for all } u \in X.\end{aligned}$$

Using this fact and the estimate (4.2.8), we obtain

$$\mu\|u\|^2 \leq \mathcal{L}(u(t)) + C_\mu \leq \mathcal{L}(u_0) + C_\mu \leq C,$$

which implies that the solution $u(t)$ is globally defined.
We now prove the continuity of the solution with respect to initial data. For any $T > 0$, let u and v be two solutions of (4.3.10) on $[0, T)$ starting from u_0 and, respectively, v_0. We then have

$$(u - v)_t = \gamma\mathcal{A}_\varepsilon(u - v) + h_\varepsilon(u) - h_\varepsilon(v), \quad 0 < t < T.$$

Taking the L^2-scalar product of this equation with $(u-v)$ and using Lemma 4.11 and Lemma 4.12, we find

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|u-v\|^2 &= \gamma < \mathcal{A}_\varepsilon(u-v),\, u-v > + < h_\varepsilon(u) - h_\varepsilon(v),\, u-v > \\ &\le \|h_\varepsilon(u) - h_\varepsilon(v)\|\|u-v\| \\ &\le 2\|f(u+M) - f(v+M)\|\|u-v\| \\ &\le C\|u-v\|^2,\end{aligned}$$

where C is a positive constant depending on T. The last inequality implies

$$\|u(t) - v(t)\|^2 \le e^{2CT}\|u_0 - v_0\|,$$

which completes the proof of the theorem. □

Remark 4.14 The family of solution operators, $\{T(t) : X \to X,\ t \ge 0\}$, given by $T(t)u_0 = u(x,\, t;\, u_0)$, define a continuous semigroup on X, and the functional $\mathcal{L}(u)$ is a Lyapunov function for the semigroup.

4.4 The nonlocal viscous Cahn-Hilliard equation

In this section we shall consider the equation

$$(1-\alpha)u_t = -A_\varepsilon(\gamma A_\varepsilon u - f(u) - \alpha u_t), \quad x \in \Omega, \tag{4.4.1}$$

or, written in an equivalent form,

$$(1-\alpha)u_t = -A_\varepsilon(N_\varepsilon^\gamma u - \alpha u_t), \quad x \in \Omega, \tag{4.4.2}$$

where $0 \le \alpha \le 1$ and the operators A_ε and N_ε^γ are given by (3.3.3) and (4.3.8), respectively. This equation is considered together with the initial condition

$$u(x,\, 0) = u_0(x), \quad x \in \Omega. \tag{4.4.3}$$

One can easily check that this equation conserves mass, that is

$$\frac{1}{|\Omega|}\int_\Omega u(x,\, t)\, dx = \frac{1}{|\Omega|}\int_\Omega u_0(x)\, dx = M, \quad \text{for all } t > 0. \tag{4.4.4}$$

Because of the term $A_\varepsilon u_t$ we shall regard this equation as the *nonlocal viscous Cahn-Hilliard equation.* A motivation for considering an equation of this sort is that (4.4.1) is the analogue of the viscous Cahn-Hilliard equation, derived by Novick-Cohen [80]. Note that if we take $\alpha = 0$, we get (4.3.1), and for $\alpha = 1$, the result is (4.2.1). We shall formulate (4.4.1)-(4.4.3) as an ordinary differential equation in a Banach space and apply the semigroup theory to prove existence and uniqueness results. For $\alpha = 0$ or 1 the existence and uniqueness theory for (4.4.1) has been carried out in the previous two sections. Following the idea of [59], we can rewrite (4.4.1) in a more useful way, that is

$$(1-\alpha)u_t = A_\varepsilon \eta, \qquad x \in \Omega, \quad t > 0, \tag{4.4.5}$$

$$\alpha u_t = \gamma A_\varepsilon u - f(u) + \eta + C, \qquad x \in \Omega, \quad t > 0, \tag{4.4.6}$$

with $\eta \in X$ and C a constant which can be determined by applying the condition (4.4.4) to (4.4.6). We find

$$C = \frac{1}{|\Omega|}\int_\Omega (\eta(x) + C)\,dx = \frac{1}{|\Omega|}\int_\Omega f(u(x))\,dx.$$

Let $\mathcal{S}_\varepsilon : X \to X$ be the solution operator given by the problem (4.3.2). We now introduce the invertible operator $B_\varepsilon^\alpha : X \to X$, defined by

$$B_\varepsilon^\alpha u = \alpha u + (1-\alpha)\mathcal{S}_\varepsilon u. \tag{4.4.7}$$

Translating the variable u from u to $u + M$, (4.4.5) and (4.4.6) become

$$B_\varepsilon^\alpha u_t = \gamma A_\varepsilon u - f(u+M) + \frac{1}{|\Omega|}\int_\Omega f(u+M)\,dx, \quad x \in \Omega, \quad t > 0. \tag{4.4.8}$$

It follows that the problem (4.4.1)-(4.4.3) may be written as the abstract initial value problem

$$(NV) \quad \begin{cases} u_t = \gamma \mathcal{B}_\varepsilon^\alpha u + \psi(u), & t > 0, \\ u(0) = u_0, \end{cases}$$

where

$$\mathcal{B}_\varepsilon^\alpha u = (B_\varepsilon^\alpha)^{-1} A_\varepsilon u, \tag{4.4.9}$$

and

$$\psi(u) = (B_\varepsilon^\alpha)^{-1}\left(\frac{1}{|\Omega|}\int_\Omega f(u+M)\,dx - f(u+M)\right). \tag{4.4.10}$$

(The fact that B_ε^α is invertible will be shown later, in Lemma 4.17.)

Before starting the semigroup approach for (NV), let us define the following scalar product on X:

$$< u, v >_1 = < -A_\varepsilon u, v >, \quad u, v \in X, \tag{4.4.11}$$

which induces the norm

$$\|u\|_1^2 = < -A_\varepsilon u, u > \quad (\equiv \frac{1}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u(y)-u(x)]^2 dydx). \tag{4.4.12}$$

Using the properties of A_ε proved in Lemma 4.1, one can easily check that, indeed, $\|\cdot\|_1$ defines a norm on X. From (4.4.12) and Lemma 4.1 we get

$$\|u\|_1 \leq \sqrt{2}\,\|u\|, \quad \text{for all } u \in X. \tag{4.4.13}$$

Using this inequality, one can prove

Lemma 4.15 *The linear operator $A_\varepsilon : X \to X$ is bounded, non-positive and self-adjoint with respect to the scalar product $< \cdot, \cdot >_1$.*

Proof. Indeed, we have

$$< A_\varepsilon u, u >_1 = < A_\varepsilon u, -A_\varepsilon u > = -\|A_\varepsilon u\|^2, \quad \text{for all } u \in X,$$

which proves the non-positiveness of A_ε. The continuity follows from the following arguments

$$\begin{aligned}
\|A_\varepsilon u\|_1^2 &\leq 2\,\|A_\varepsilon u\|^2 \\
&= 2\int_\Omega \left[\int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))\,dy\right]^2 dx \\
&= 2\int_\Omega \left[\int_\Omega J_\varepsilon^{1/2}(|x-y|)J_\varepsilon^{1/2}(|x-y|)(u(y)-u(x))\,dy\right]^2 .dx \qquad (4.4.14)\\
&\leq 2\int_\Omega \left[\left(\int_\Omega J_\varepsilon(|x-y|)\,dy\right)\left(\int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))^2\,dy\right)\right] dx \\
&\leq 2\int_\Omega \left[\left(\int_{\mathbb{R}} J_\varepsilon(|x-y|)\,dy\right)\left(\int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))^2\,dy\right)\right] dx \\
&= 2\int_\Omega \int_\Omega J_\varepsilon(|x-y|)(u(y)-u(x))^2\,dy\,dx \\
&= 4\,\|u\|_1^2,
\end{aligned}$$

where in (4.4.14) we have used the Cauchy-Schwarz formula. The self-adjointness follows from the similar property of A_ε with respect to the L^2-scalar product, proved in Lemma 4.1. □

Remark 4.16 The boundedness of A_ε in $\|\cdot\|_1$ implies that

$$\|A_\varepsilon w\|_1 \leq C\|w\|_1, \qquad \text{for all } w \text{ solutions of (4.3.2)},$$

which is equivalent to

$$\|u\|_1 \leq C|||u|||, \quad u \in X. \tag{4.4.15}$$

Let us use the notation

$$|u|_B^2 = < B_\varepsilon^\alpha u, u >, \quad \text{for all } u \in X. \tag{4.4.16}$$

For all $u \in X$, we have

$$\begin{aligned} |u|_B^2 \equiv < B_\varepsilon^\alpha u, u > &= < \alpha u + (1-\alpha)\mathcal{S}_\varepsilon u, u > \\ &= \alpha\|u\|^2 + (1-\alpha)|||u|||^2. \end{aligned} \tag{4.4.17}$$

The relations (4.4.13), (4.4.15) and (4.4.17) imply

$$\|u\|_1 \leq C|u|_B, \quad \text{for all } u \in X. \tag{4.4.18}$$

Lemma 4.17 *For $\alpha \in (0, 1]$ the linear operator $B_\varepsilon^\alpha : X \to X$ is non-negative, self-adjoint, invertible, and has a bounded inverse in X (with respect to the norm $\|\cdot\|$ on X).*

Proof. The first property follows from (4.4.17). The self-adjointness follows from

$$\begin{aligned} < B_\varepsilon^\alpha u, v > &= \alpha < u, v > +(1-\alpha) < \mathcal{S}_\varepsilon u, v > \\ &= \alpha < u, v > +(1-\alpha) \ll u, v \gg \\ &= \alpha < u, v > +(1-\alpha) < u, \mathcal{S}_\varepsilon v > \\ &= < u, \alpha v + (1-\alpha)\mathcal{S}_\varepsilon v > \\ &= < u, B_\varepsilon^\alpha v >, \end{aligned}$$

for all $u, v \in X$, $\alpha \in [0, 1]$. From (4.4.17) we get that

$$B_\epsilon^\alpha u = 0 \implies u = 0,$$

so B_ϵ^α possesses an inverse $(B_\epsilon^\alpha)^{-1}$ defined on X. To show that the inverse is bounded for each $\alpha > 0$, we will prove that there exists a positive constant C such that

$$\|B_\epsilon^\alpha u\| \geq C\|u\|, \quad \text{for all } u \in X.$$

We have

$$\begin{aligned}
\|B_\epsilon^\alpha u\|^2 &= < \alpha u + (1-\alpha)\mathcal{S}_\epsilon u,\ \alpha u + (1-\alpha)\mathcal{S}_\epsilon u > \\
&= \alpha^2\|u\|^2 + 2\alpha(1-\alpha) < u,\ \mathcal{S}_\epsilon u > + (1-\alpha)^2\|\mathcal{S}_\epsilon u\| \\
&\geq \alpha^2\|u\|^2 + 2\alpha(1-\alpha)\|\|u\|\|^2 \\
&\geq C\|u\|^2, \qquad \text{if } \alpha \neq 0,
\end{aligned}$$

which completes the proof. □

Lemma 4.18 *If $f : L^2(\Omega) \to L^2(\Omega)$ is locally Lipschitz, then the operator $\psi : X \to X$ given by (4.4.10) is locally Lipschitz in the norm $\|\cdot\|$.*

Proof. Denote by g the operator

$$g(u) = \frac{1}{|\Omega|}\int_\Omega f(u(x) + M)\,dx - f(u + M).$$

Using the boundedness of $(B_\epsilon^\alpha)^{-1}$ in the norm $\|\cdot\|$, for any $u, v \in X$ we have

$$\begin{aligned}
\|\psi(u) - \psi(v)\| &= \|(B_\epsilon^\alpha)^{-1}[g(u) - g(v)]\| \\
&\leq C\|g(u) - g(v)\|.
\end{aligned}$$

The application of Lemma 4.2 completes the proof of the lemma. □

We can now prove the existence and uniqueness theorem.

Theorem 4.19 *We assume that J satisfies $(\mathcal{H}_1)$, the function $f : L^2(\Omega) \to L^2(\Omega)$ is locally Lipschitz and satisfies (3.6.26). Then, for every u_0 given in X, the initial-value problem (NV) possesses a unique solution u which belongs to $C([0, T];\ X)$, for all $T > 0$, and depends continuously on the initial data. The $\mathcal{L}(u)$ defined by (3.3.9) is the Lyapunov function for the generated semigroup.*

Proof. Using the previous two lemmas, we get the existence and uniqueness of a local solution $u(t)$ defined on a maximal interval $[0, T)$. To prove the global existence of this solution we shall need some a priori bounds of $u(t)$ on $[0, T)$. We observe that for functions of zero-mass we can rewrite the functional $\mathcal{L}(u)$ given by (3.3.9) as

$$\mathcal{L}(u) = \frac{\gamma}{2}\|u\|_1^2 + \int_\Omega F(u(x) + M)\, dx. \tag{4.4.19}$$

Let us take the L^2-inner product of (4.4.8) with u_t. We get

$$\begin{aligned} < B_\epsilon^\alpha u_t,\, u_t > &= -\gamma < -A_\epsilon u,\, u_t > - < f(u+M),\, u_t > \\ &= -\frac{\gamma}{2}\frac{d}{dt}\|u\|_1^2 - \frac{d}{dt}\int_\Omega F(u+M)\, dx, \end{aligned}$$

valid for all $u \in X$. We obtain

$$\frac{d}{dt}\mathcal{L}(u) = -|u_t|_B^2 \leq 0, \quad \text{for all } u \in X, \tag{4.4.20}$$

and thus, $\mathcal{L}(u(t))$ is decreasing in time, so we have

$$\mathcal{L}(u(t)) \leq \mathcal{L}(u_0) \leq C, \quad \text{for all } t > 0. \tag{4.4.21}$$

Using the estimates (4.2.8) and (4.4.13), we conclude that for all $\mu > 0$, there exist some positive constants $C_{1\mu}$ and $C_{2\mu}$ such that

$$\int_\Omega F(u)\, dx \geq C_{1\mu}\|u\|_1^2 - C_{2\mu}, \quad \text{for all } u \in X,$$

which implies

$$\mathcal{L}(u) \geq C_1\|u\|_1^2 - C_2, \quad \text{for all } u \in X,$$

for some constants C_1 and C_2. The previous inequality and (4.4.21) yields the a priori estimate

$$\|u(t)\|_1 \leq C, \quad \text{for all } t > 0,$$

which establishes the global existence of the solution to (NV).

If $u, v \in X$ are two solutions to (NV) starting from u_0 and v_0, respectively, then

$$B_\epsilon^\alpha(u-v)_t = \gamma A_\epsilon(u-v) + f(v+M) - f(u+M) + \frac{1}{|\Omega|}\int_\Omega [f(u+M) - f(v+M)]\, dy.$$

Let us consider firstly the case $\alpha \in (0, 1]$. Taking the L^2-inner product of this with $(u - v)$ and using the fact that A_ε is non-positive in X, we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}|u-v|_B^2 &= < A_\varepsilon(u-v),\, u-v > - < f(u+M) - f(v+M),\, u-v > \\ &\leq - < f(u+M) - f(v+M),\, u-v > \\ &\leq \|f(u+M) - f(v+M)\|\|u-v\| \\ &\leq C\|u-v\|^2 \\ &\leq C|u-v|_B^2,\end{aligned}$$

which implies that

$$|u(t) - v(t)|_B \leq C(T)|u_0 - v_0|_B, \qquad \text{for } t \in [0, T).$$

If $\alpha = 0$, then the property is proved in Theorem 4.13. Clearly, using (4.4.20) and the fact that $\mathcal{L}(u)$ is bounded from below (since $F(u)$ is so), we conclude that the functional given by (4.4.19) is a Lyapunov function for the semigroup. □

4.5 Stationary solutions

For definiteness, we shall take $f(u) = \alpha_2 u^3 + \alpha_1 u^2 - u$, where α_1, α_2 are some constants. An equilibrium point u for (4.4.1) is a mass-conserving extreme value of $\mathcal{L}$, that is,

$$u \in L^2(\Omega), \text{ such that } \frac{d}{dh}\mathcal{L}(u + hv)|_{h=0} = 0, \qquad \text{for all } v \in L^2(\Omega),$$

and

$$\frac{1}{|\Omega|}\int_\Omega u(x)\,dx = M. \tag{4.5.1}$$

Clearly, since the free energy functional $\mathcal{L}(u)$ given by (3.3.9) is independent of α, so will be the set of equilibria. Thus, we have the following

Lemma 4.20 *The problem of finding critical points of the functional $\mathcal{L}(u)$ over*

$\{u \in L^2(\Omega),\ \frac{1}{|\Omega|}\int_\Omega u(x) = M\}$ *is equivalent to the problem:*

$$(S)\quad \begin{cases} \gamma A_\varepsilon u - f(u) + \dfrac{1}{|\Omega|}\displaystyle\int_\Omega f(u(x))dx = 0, \quad x \in \Omega, \\ \dfrac{1}{|\Omega|}\displaystyle\int_\Omega u(x)dx = M. \end{cases}$$

Proof. This follows immediately, since the constrained gradient of $\mathcal{L}(u)$ with respect to the inner product $<,>$ is

$$\mathrm{grad}_{\mathcal{M}}\mathcal{L}(u) = -\gamma A_\varepsilon u + f(u) - \frac{1}{|\Omega|}\int_\Omega f(u(x))dx.$$

□

Remark 4.21 Let us consider the equation obtained from $(S)_1$ by setting γ to zero. We get

$$f(u) - \int_\Omega f(u(y)\,dy = 0,\ x \in \Omega. \tag{4.5.2}$$

Since A_ε is a bounded operator, the $\mathcal{O}(\gamma)$ term in $(S)_1$ is a regular perturbation of (4.5.2). Because (4.5.2) possesses an uncountable number of solutions which satisfy the mass constraint $(S)_2$, the number of solutions of (S) will also be uncountable if γ is small enough. It is well known that the situation is different in the viscous Cahn-Hilliard case. It was shown in [103] that (2.2.15) possesses a finite number of steady states, which Grinfeld and Novick-Cohen [58] have counted.

By translating the order parameter u, problem (S) reduces to

$$(SO)\quad \begin{cases} \gamma A_\varepsilon u - f(u+M) + \dfrac{1}{|\Omega|}\displaystyle\int_\Omega f(u(x)+M)\,dx = 0, \quad x \in \Omega, \\ \displaystyle\int_\Omega u(x)dx = 0. \end{cases}$$

In the particular case $\gamma = 0$, $\alpha_1 = 0$ and $\alpha_2 = 1$, we have

$$F(u) = \frac{1}{4}u^4 - \frac{1}{2}u^2,$$

and the steady state problem reduces to

$$\text{Minimize} \quad \int_\Omega F(u(x))\,dx \quad - \quad \text{over all } u \in L^2(\Omega), \tag{4.5.3}$$

subject to (4.5.1). Following [20], minimizers are either constant M (*single-phase solutions*) or piecewise constant (*two-phase solutions*), where in the latter case they have the form:

$$u(x) = \begin{cases} -1, & x \in \Omega_1 \\ \\ +1, & x \in \Omega_2, \end{cases}$$

where Ω_1, Ω_2 are disjoint measurable sets, such that $\Omega_1 \bigcup \Omega_2 = \Omega$.

Obviously, if the mass $|M| \geq 1$ a two-phase solution of (4.5.3) is not possible, thus the minimizer is the single phase solution $u(x) \equiv M$.

In what follows we shall be concerned about solutions of (SO) with $\gamma > 0$. For simplicity we set $|\Omega| = 1$. We start with the following

Proposition 4.22 *If $\alpha_2 > 0$, then the set of equilibria is bounded in X.*

Proof. We multiply $(SO)_1$ by u and then integrate with respect to x over Ω. Using the monotonicity property of A_ε and $(SO)_2$, we get

$$\int_\Omega f(u+M)u\,dx \leq 0,$$

which is equivalent to

$$\int_\Omega [\alpha_2 u^2 + (3\alpha_2 M + \alpha_1)u + 3\alpha_2 M^2 + 2\alpha_1 M - 1\,]\,u^2\,dx \leq 0, \tag{4.5.4}$$

implying

$$\alpha_2 u^2 + (3\alpha_2 M + \alpha_1)u + 3\alpha_2 M^2 + 2\alpha_1 M - 1 \leq 0, \tag{4.5.5}$$

from which we get that $\|u\|_\infty$, and consequently $\|u\|$, can only be bounded (because $\alpha_2 \gneq 0$). □

Theorem 4.23 *If $|M|$ is large enough, then the steady state problem (SO) has only the trivial solution $u \equiv 0$ (i.e., $u \equiv M$ is the only solution of (S)).*

Proof. Indeed, if $|M|$ is large enough, then we have

$$-3\alpha_2^2 M^2 - 2\alpha_1\alpha_2 M + \alpha_1^2 + 4\alpha_2 < 0,$$

which means that the left-hand side of (4.5.5) is positive defined. The inequality (4.5.4) implies that $u \equiv 0$ is the only solution of (SO). □

We can also prove the following

Theorem 4.24 *Assume $\alpha_2 > 0$, J satisfies $(\mathcal{H}_1)$, and the mass M is given. Then for γ large enough the steady state problem (SO) has only the trivial solution $u \equiv 0$.*

Proof. If u is a solution of (SO), then

$$0 = \gamma \int_\Omega J_\varepsilon(|x-y|)[u(x)-u(y)]\,dy + f(u+M) - \int_\Omega f(u+M)\,dy. \qquad (4.5.6)$$

Multiplying (4.5.6) by $u(x)$ and then integrating over Ω,

$$\begin{aligned} 0 &= \gamma \int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u^2(x)-u(x)u(y)]\,dydx + \int_\Omega f(u(x)+M)u(x)\,dx \\ &= \frac{\gamma}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u(x)-u(y)]^2\,dydx + \\ &\quad + \int_\Omega [\alpha_2 u^2(x) + (3\alpha_2 M + \alpha_1)u(x) + 3\alpha_2 M^2 + 2\alpha_1 M - 1\,]\,u^2(x)\,dx \\ &\geq \frac{\gamma}{2}\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u(x)-u(y)]^2\,dydx + C_1\|u\|^2 - C_2, \qquad (4.5.7) \end{aligned}$$

valid for all $\gamma > 0$, where C_1, C_2 are positive constants depending on M, α_1, α_2. One can easily observe that the inequality (4.5.7) is always satisfied by $u \equiv 0$. Let us suppose that the problem (SO) has also a nontrivial solution u^*. Then we have

$$\|u^*\|^2 = \zeta^2 > 0,$$

and

$$\int_\Omega \int_\Omega J_\varepsilon(|x-y|)[u^*(x)-u^*(y)]^2\,dydx = \mu^2 > 0. \qquad (\text{since } J_\varepsilon(\cdot) > 0)$$

The inequality (4.5.7) applied to u^* implies

$$0 > \frac{\gamma}{2}\mu^2 + C_1\zeta^2 - C_2. \qquad (4.5.8)$$

Obviously, by choosing

$$\gamma > \frac{2}{\mu^2}(C_2 - C_1\zeta^2),$$

such nontrivial solutions do not exist. □

Remark 4.25 The last two results also hold for the equilibrium solutions of (2.2.15) (see [103]). This means that (4.4.1) and (2.2.15) have the same solution for large enough values of $|M|$ or strength parameter (this is γ for (4.4.1), and ϵ for (2.2.15)).

4.6 Linear analysis

We prove now that if the mass M lies outside the spinodal region, that is $f'(M) > 0$, then the trivial solution $u \equiv 0$ of (SO) is linearly stable. In order to simplify the calculation, we shall work on $\mathbb{R}$ rather than on Ω. In this case, the problem (SO) can be written as:

$$(SOR) \quad \begin{cases} \gamma A_\varepsilon u - f(u+M) + \int_{\mathbb{R}} f(u(x)+M)\,dx = 0, \quad x \in \mathbb{R}, \\ \int_{\mathbb{R}} u(x)dx = 0, \end{cases}$$

where

$$A_\varepsilon u(x) = \int_{\mathbb{R}} J_\varepsilon(|x-y|)(u(y)-u(x))\,dy, \quad x \in \mathbb{R}. \tag{4.6.1}$$

Let $L_\varepsilon^\gamma u$ be the linearization of the left-hand side of $(SOR)_1$ about $u \equiv 0$, that is

$$L_\varepsilon^\gamma u(x) = \gamma \int_{\mathbb{R}} J_\varepsilon(|x-y|)[u(y)-u(x)]dy - f'(M)u(x), \quad x \in \mathbb{R}.$$

Firstly, we investigate the spectrum of L_ε^γ. Since

$$\begin{aligned}(L_\varepsilon^\gamma - \lambda)\phi &= \gamma \int_{\mathbb{R}} J_\varepsilon(|x-y|)\phi(y)\,dy - [\gamma + f'(M) + \lambda]\phi \\ &= [\gamma + f'(M) + \lambda]\left[\frac{\gamma}{\gamma + f'(M) + \lambda}\int_{\mathbb{R}} J_\varepsilon(|x-y|)\phi(y)\,dy - \phi\right],\end{aligned}$$

we see that $L_\varepsilon^\gamma - \lambda$ is invertible for

$$\gamma \|J_\varepsilon\|_{L^1(\mathbb{R})} < |\lambda + f'(M) + \gamma|.$$

Since $\|J_\varepsilon\|_{L^1(\mathbb{R})} = 1$, the spectrum of L_ε^γ satisfies

$$\sigma(L_\varepsilon^\gamma) \subset \{\lambda : |\lambda + f'(M) + \gamma| \leq \gamma\}.$$

We see now that for $f'(M) > 0$ the spectrum of L_ε^γ lies in the left-half plane, and thus $u \equiv 0$ is linearly stable.

In what follows we would like to get the *dispersion relation* (the relationship between the wavelength of a mode and its corresponding growth rate) imposed

by (4.4.1). Since $\alpha = 1$ is a critical case for (4.4.1), we shall discuss the case $\alpha \in [0, 1)$ firstly. Linearizing (4.4.1) about $u \equiv M$, one obtains

$$
\begin{aligned}
&(1-\alpha)u_t = \\
&= -A_\varepsilon(L_\varepsilon^\gamma u - \alpha u_t) \\
&= -A_\varepsilon(L_\varepsilon^\gamma u) + \alpha A_\varepsilon(u_t) \\
&= \int_{\mathbb{R}} J_\varepsilon(|x-y|)[L_\varepsilon^\gamma u(x) - L_\varepsilon^\gamma u(y)]dy + \alpha \int_{\mathbb{R}} J_\varepsilon(|x-y|)[u_t(y) - u_t(x)]dy \\
&= \int_{\mathbb{R}} J(|w|)[L_\varepsilon^\gamma u(x) - L_\varepsilon^\gamma u(x+\varepsilon w)]dw + \alpha \int_{\mathbb{R}} J(|w|)[u_t(x+\varepsilon w) - u_t(x)]dw \\
&= \gamma \int_{\mathbb{R}} J(|w|) \left\{ \int_{\mathbb{R}} J(|\eta|)[u(x+\varepsilon\eta) - u(x)]d\eta \right\} dw - \\
&\qquad -\gamma \int_{\mathbb{R}} J(|w|)\{ \int_{\mathbb{R}} J(|\eta|)[u(x+\varepsilon\eta+\varepsilon w)) - u(x+\varepsilon w)]d\eta\}dw \qquad (4.6.2) \\
&+f'(M) \int_{\mathbb{R}} J(|w|)[u(x+\varepsilon w) - u(x)]dw + \alpha \int_{\mathbb{R}} J(|w|)[u_t(x+\varepsilon w) - u_t(x)]dw.
\end{aligned}
$$

We now look for solutions of the form $u(x, t) = e^{\lambda t + ikx}$. Such solutions are possible if and only if

$$
\begin{aligned}
(1-\alpha)\lambda = -\gamma \left(\int_{\mathbb{R}} J(|w|)(1-\cos(kw\varepsilon))dw \right)^2 \\
-(f'(M) + \alpha\lambda) \int_{\mathbb{R}} J(|w|)(1-\cos(kw\varepsilon))dw. \qquad (4.6.3)
\end{aligned}
$$

If we denote by

$$
h(k, \varepsilon) = \int_{\mathbb{R}} J(|w|)(1-\cos(kw\varepsilon))dw, \qquad (4.6.4)
$$

then we can write (4.6.3) as

$$
(1-\alpha)\lambda = -h(k, \varepsilon)[f'(M) + \alpha\lambda + \gamma h(k, \varepsilon)].
$$

or

$$
[1 - \alpha + \alpha h(k, \varepsilon)]\, \lambda(k) = -h(k, \varepsilon)[f'(M) + \gamma h(k, \varepsilon)], \quad \alpha \in [0, 1). \qquad (4.6.5)
$$

The relation (4.6.5) represents the dispersion relation for (4.4.1) with $\alpha \in [0, 1)$. Note that $h(k, \varepsilon)$ are the eigenvalues of the operator $-A_\varepsilon$, which are bounded (they belong to the interval $[0, 2]$). Indeed, if ν is an eigenvalue of $-A_\varepsilon$, then ν satisfies

$$
\nu\, u(x) = -\int_{\mathbb{R}} J(|w|)(u(x) - u(x+\epsilon w))\, dw.
$$

If we are looking for solutions of the form $u(x, t) = e^{ikx}$, we get

$$\begin{aligned}\nu(k) &= \int_{\mathbb{R}} J(|w|)(1 - e^{ik\epsilon w})\, dw \\ &= \int_{\mathbb{R}} J(|w|)(1 - \cos(k\epsilon w))\, dw = h(k, \epsilon).\end{aligned}$$

In the special case $\alpha = 1$, equation (4.4.1) reduces to

$$u_t = \gamma A_\varepsilon u - f(u) + \int_{\mathbb{R}} f(u(x))\, dx, \quad x \in \mathbb{R},$$

with A_ε given by (4.6.1). The linearized equation about $u \equiv M$ is

$$u_t = L_\varepsilon^\gamma u, \quad x \in \mathbb{R},$$

and the dispersion relation is

$$\lambda(k) = -\gamma h(k, \epsilon) - f'(M). \tag{4.6.6}$$

Remark 4.26 If the mass M lies outside the spinodal region, then $f'(M) > 0$, and relations (4.6.5) and (4.6.6) imply that the trivial solution $u \equiv M$ is linearly stable in the L^∞-norm, regardless the value of $\alpha \in [0, 1]$.

Remark 4.27 If we take $\gamma = 1$ and approximate $cos(kw\varepsilon)$ by the first two terms of the Taylor series expansion, then from (4.6.5) and (4.6.6) we find the dispersion relation for the viscous Cahn-Hilliard (2.2.15) equation (after time scaling by ε^2). For $\alpha \in [0, 1)$ this is

$$(1 - \alpha + \alpha\pi^2 k^2)\, \lambda_k = -\pi^2 k^2 (f'(M) + \varepsilon^2 \pi^2 k^2), \tag{4.6.7}$$

and for $\alpha = 1$,

$$\lambda_k = -\epsilon^2 \pi^2 k^2 - f'(M). \tag{4.6.8}$$

Note that due to the boundary conditions (2.2.17) the eigenvalues given by (4.6.7) or (4.6.8) correspond only to integer values of k. In Figure 4.1, we have plotted the continuous curves which contain these eigenvalues, for different values of α. One can see that the curves corresponding to $\alpha \in [0, 1)$ are "humped", while for $\alpha = 1$ the eigenvalues are strictly decreasing. For each value of α in $[0, 1)$, there is generically a unique fastest-growing mode, and the wavelength of this mode in

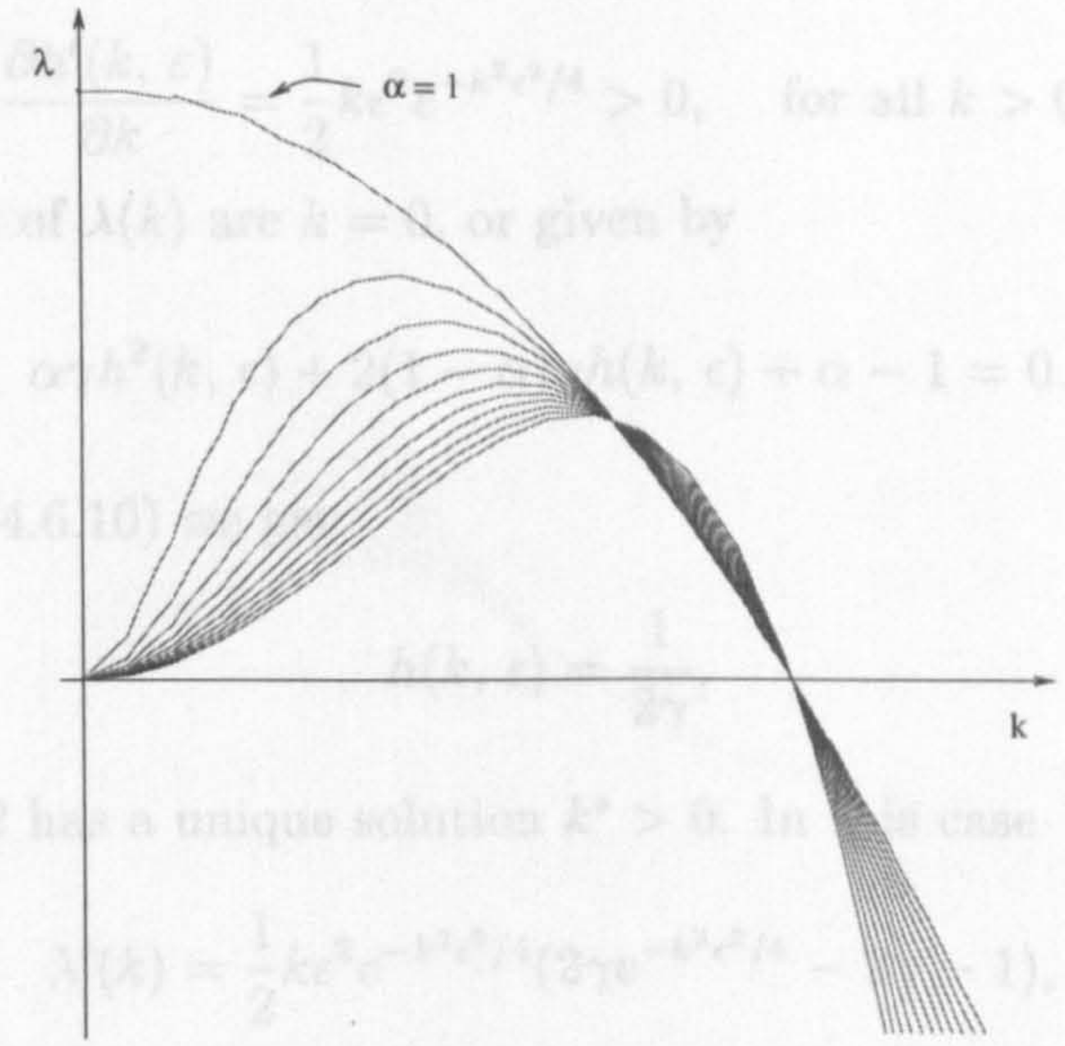

Figure 4.1: The dispersion relation (4.6.7) for different values of $\alpha \in [0, 1]$.

$\mathcal{O}(\epsilon)$ as $\epsilon \to 0$ (see [57]). All eigenvalues of (4.3.1) approach $-\infty$ as $k \to \infty$. In [57] Grant proved that the fastest-growing mode will dominate the behaviour of most solutions of the Cahn-Hilliard equation (2.2.19) with initial values that are small perturbations from the constant mass solution.

We are interested to see whether one can find a fastest growing mode in the case of (4.6.5).

We shall discuss this problem only in a particular case, that is

$$J(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}, \quad f(u) = u^3 - u, \quad \text{and } M = 0.$$

In this case we have

$$h(k, \epsilon) = 1 - e^{-k^2\epsilon^2/4} \in [0, 1), \quad f'(M) = -1.$$

Once again, we discuss firstly the case $\alpha \in [0, 1)$. By differentiating (4.6.5) with respect to k and then multiplying the result by $(1 - \alpha + \alpha h(k, \varepsilon))$, we obtain

$$[1-\alpha+\alpha h(k, \varepsilon)]^2 \frac{d\lambda}{dk} = -\frac{\partial h'(k, \varepsilon)}{\partial k}[\alpha\gamma h^2(k, \epsilon)+2\gamma(1-\alpha)h(k, \epsilon)+\alpha-1]. \quad (4.6.9)$$

Since

$$\frac{\partial h'(k,\,\varepsilon)}{\partial k} = \frac{1}{2}k\epsilon^2 e^{-k^2\epsilon^2/4} > 0, \quad \text{for all } k > 0,$$

the critical points of $\lambda(k)$ are $k = 0$, or given by

$$\alpha\gamma h^2(k,\,\epsilon) + 2(1-\alpha)\gamma h(k,\,\epsilon) + \alpha - 1 = 0. \tag{4.6.10}$$

For $\alpha = 0$, from (4.6.10) we get

$$h(k,\,\epsilon) = \frac{1}{2\gamma},$$

which for $\gamma > 1/2$ has a unique solution $k^* > 0$. In this case

$$\lambda'(k) = \frac{1}{2}k\epsilon^2 e^{-k^2\epsilon^2/4}(2\gamma e^{-k^2\epsilon^2/4} - 2\gamma - 1),$$

which is positive for $k < k^*$ and negative for $k > k^*$. This means that k^* is a local maximum point for $\lambda(k)$, which corresponds to the fastest growing mode. In this case $k = 0$ is a local minimum point for λ.

Consider now $\alpha \in (0,\,1)$. The discriminant of (4.6.10) is

$$\Delta = 4\gamma(1-\alpha)[\alpha + (1-\alpha)\gamma],$$

which is positive. Solving (4.6.10) with respect to h we get the solutions

$$h_1 = \frac{(\alpha-1)}{\alpha} - \frac{1}{\alpha\gamma}[\gamma(1-\alpha)(\alpha+\gamma-\alpha\gamma)]^{\frac{1}{2}} < 0, \quad \text{and}$$

$$h_2 = \frac{(\alpha-1)}{\alpha} + \frac{1}{\alpha\gamma}[\gamma(1-\alpha)(\alpha+\gamma-\alpha\gamma)]^{\frac{1}{2}} > 0.$$

Thus, we may find at most one solution in $[0,\,1)$. We have $h_2 \in [0,\,1)$ if $\gamma > (1-\alpha)/(2+\alpha)$. Let us fix $\alpha \in (0,\,1)$. For γ small enough, (4.6.10) has no solution in $[0,\,1]$, which means that $k = 0$ is the only critical point of $\lambda(k)$. Since $\lambda''(0) > 0$, $k = 0$ is a local minimum point.

For large enough γ, the equation (4.6.10) has exactly one solution in $[0,\,1]$, that is h_2. Due to the continuity and strict monotonicity of $h(k,\,\epsilon)$, we get a unique positive value of k, denoted by k^*, such that $h(k,\,\epsilon) = h_2$. Since $\lambda'(k)$ is positive for $k < k^*$ and negative for $k > k^*$, the value k^* is a local maximum point for $\lambda(k)$. In Figure 4.2 we plotted the dispersion relation (4.6.5) for different

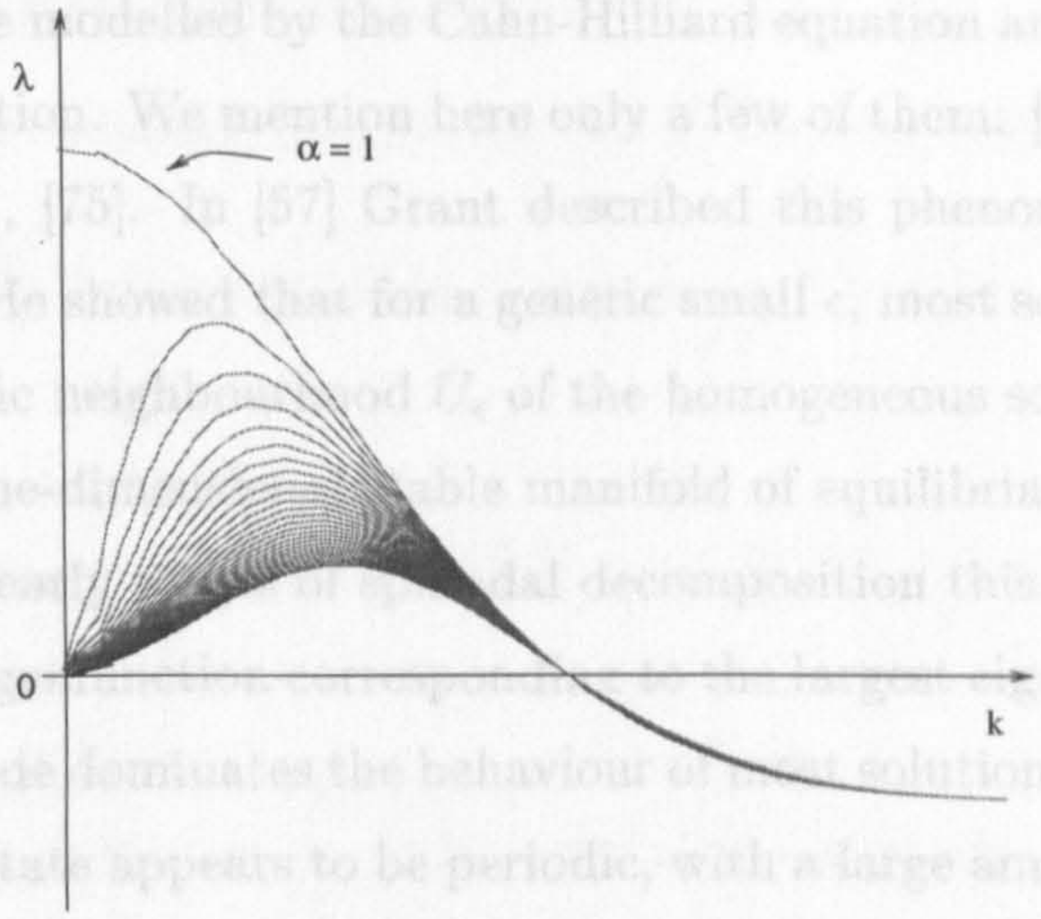

Figure 4.2: The dispersion relation (4.6.5) for different values of $\alpha \in [0, 1]$.

values of α. We see that the curves corresponding to $\alpha \in [0, 1)$ are "humped", and for $\alpha = 1$ the function λ is a decreasing function of k. Generically, for large enough values of γ there is a fastest-growing mode.

For $\alpha = 1$ the dispersion relation is given by (4.6.6). Differentiating this relation with respect to k, we get

$$\lambda'(k) = -\frac{\gamma}{2} k\epsilon^2 e^{-k^2\epsilon^2/4},$$

whence $k = 0$ is the only critical value, which is the global maximum point for $\lambda(k)$.

As shown in Figure 4.2, the function $\lambda(k)$ is not "humped" for $\alpha = 1$, but all the functions $\lambda(k)$ with $\alpha \in [0, 1)$ are bounded, unlike the eigenvalues of (2.2.15).

Remark 4.28 As already mentioned in Section 2.2.3, the Cahn-Hilliard equation can be used to model phase separation in molten binary alloys. When a spatially homogeneous molten binary mixture is suddenly quenched below the critical temperature, then a fine-grained decomposition into two distinct phases can be observed, a phenomenon which is known as *spinodal decomposition*. There are many papers in the literature dealing with spinodal decomposition, how this

phenomenon can be modelled by the Cahn-Hilliard equation and numerical simulations of this equation. We mention here only a few of them: [15], [16], [17], [35], [36], [57], [65], [74], [75]. In [57] Grant described this phenomenon in the one-dimensional case. He showed that for a generic small ϵ, most solutions of (2.2.19) starting in a specific neighbourhood U_ϵ of the homogeneous solution $u \equiv M$ will stay close to the one-dimensional stable manifold of equilibria. It was rigorously shown that in the early stages of spinodal decomposition this unstable manifold is tangent to the eigenfunction corresponding to the largest eigenvalue, and so the fastest-growing mode dominates the behaviour of most solutions originating in U_ϵ. A solution in this state appears to be periodic, with a large amplitude. It is interesting to note that practically every random perturbation yields the same result. After spinodal decomposition, the solution of (2.2.19) will eventually coarsen to a monotonic solution (see [20]).

In higher space dimensions Grant's approach is not applicable, because it predicts patterns which are not observed in practice. Analytic and numerical studies of spinodal decomposition in higher space dimensions can be found in, among others, [35], [36], [74], [75].

In *Experiment 3* we perform numerics for the nonlocal Cahn-Hilliard equation (4.3.1) showing that spinodal decomposition can also be observed in the case.

The dispersion relation for the nonlocal Cahn-Hilliard equation can be obtained from (4.6.5) by taking $\alpha = 0$. This is

$$\lambda(k) = -h(k, \varepsilon)[f'(M) + \gamma h(k, \varepsilon)], \tag{4.6.11}$$

where $h(k, \epsilon)$ is given by (4.6.4).

4.7 Numerical analysis

In this section we carry out some numerical experiments showing that the non-coarsening phenomenon proved in the case of the non-conserving order parameter flow generated by (3.3.1) can be also observed for the mass-conserving flows generated by (NRS) and (NCH).

4.7.1 Numerical approximation

For $\Omega = (0, 1)$, the equations (4.2.1) and (4.3.1) become, respectively,

$$u_t = \frac{\gamma}{\varepsilon}\int_0^1 J(\frac{|x-y|}{\varepsilon})(u(y)-u(x))\,dy - f(u) + \int_0^1 f(u(y))dy, \quad x \in (0,1),\ t>0, \tag{4.7.1}$$

and

$$u_t = -A_\varepsilon(\gamma A_\varepsilon u - f(u)), \quad x \in (0,1),\ t>0, \tag{4.7.2}$$

with A_ε given by

$$A_\varepsilon u(x) = \int_0^1 J_\varepsilon(|x-y|)(u(y)-u(x))\,dy.$$

We use the same type of approximation scheme and notation as in Section 3.7. Let

$$\sigma = \Delta x \sum_{i=1}^{N} f(u_i),$$

and let

$$h(U) = g(U) - \sigma I_N,$$

with $g(U) = [f(u_1)\ f(u_2)\ \ldots\ f(u_N)]^T$ and $I_N = [1\ 1\ \ldots\ 1]^T$.

The equation (4.7.1) is approximated by the following system of ordinary differential equations:

$$\frac{d}{dt}U = \frac{\gamma}{\varepsilon}\Gamma U\Delta x - h(U), \tag{4.7.3}$$

where $U = [u_1\ u_2\ \ldots\ u_N]^T$, and the elements of the matrix Γ are given by (3.7.4).

We aim now to find an approximation for (4.7.2). Let us denote by V_ε^γ the vector

$$V_\varepsilon^\gamma = (\frac{\gamma}{\varepsilon}\Gamma U\Delta x - h(U))^T.$$

Then the equation (4.7.2) is approximated by the following system:

$$\frac{d}{dt}U = -\Gamma V_\varepsilon^\gamma. \tag{4.7.4}$$

4.7.2 Numerical experiments

We present here the results of the numerical simulations for the equations (4.7.1) and (4.7.2) (with $f(u) = u^3 - u$), using the above approximations. In computations we take

$$J(x) = \begin{cases} 0 & , x = 0 \\ \dfrac{10}{\sqrt{\pi}} \exp(-25x^2) & , x > 0. \end{cases}$$

Experiment 1. We fix $\epsilon = 1$, and take the initial data

$$u_0(x) = 4x(1-x)\sin(10\pi x^2), \tag{4.7.5}$$

In this case the mass $M = 0.05$ is in the spinodal region, $(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$. We use 100 lattice points to approximate the solutions of (4.2.1) and (4.3.1) for different values of γ. The results for $\gamma = 0.25$ are shown in Figures 4.3 and 4.4, where we observe a total noncoarsening of solutions to both equations. For $\gamma = 0.5$, Figures 4.5 and 4.7 show a partial coarsening of solutions. For both equations the graphs of the Lyapunov functional $\mathcal{L}(u)$ given by (3.3.9) (see Figures 4.6 and 4.8) show that, indeed, we reached equilibrium solutions, which are not continuous. We can see that for the evolution governed by (4.2.1) the steady state is reached for t slightly less than 60, when the Lyapunov function becomes minimum, and for the evolution governed by (4.3.1) the steady state is reached for $t \approx 550$.

In Figure 4.9 and Figure 4.10 we see the initial data (4.7.5) and final equilibrium solutions for a range of values of γ. One can observe that for small enough values of the parameter γ (e.g. $\gamma < 0.5$), the solutions of both (4.2.1) and (4.3.1) do not coarsen. A partial coarsening of these solutions takes place for some values of γ, e.g. $\gamma = 0.5$. For $\gamma = 1$, the solutions of these equations do coarsen to a monotonic solution, while for γ big enough solutions coarsen to the constant mass solution, which is the only steady state (as proved in Theorem 4.24).

Experiment 2. This time we fix $\gamma = 1$ and leave ε to vary. We take the same initial data as in the previous experiment and $N = 128$. In Figures 4.11 and

4.13 we represent the approximations of solutions of (4.7.1) with $\varepsilon = 0.2$, and of (4.7.2) with $\varepsilon = 0.3$, respectively. For these values of γ and ε the equilibrium solutions are only partially coarsened. Figures 4.12 and 4.14 show that these partial coarsened states minimize the Lyapunov function (3.2.3).

We plot in Figures 4.15 and 4.16 the equilibrium solutions of (4.7.1) and respectively (4.7.2), starting from u_0, for different values of ε. We can observe that for this value of γ we could not find a value of ε for which a solution converges to the constant mass solution, and this is because M lies in the spinodal region where $u \equiv M$ is unstable. We may get total non-coarsening of solutions for either small enough or big enough values of ε. In other words, one can find two values of ε, say ε^* and ε^{**} ($\varepsilon^* < \varepsilon^{**}$), so that if either $\varepsilon < \varepsilon^*$ or $\varepsilon > \varepsilon^{**}$ the solutions to (4.7.1) and (4.7.2) do not coarsen at all. If $\varepsilon = 1.5$, for example, then we find the nice coarsening of solutions of both equations to a monotonic solution.

Experiment 3. We perform a two dimensional experiment for the equation (4.2.1) on a unit square. In the approximation we use a 25×25 grid. The parameters are: $\epsilon = 1$, $\gamma = 2$, $\Delta t = 0.4$, and

$$J(x) = \begin{cases} 0 & , \quad x = 0 \\ \dfrac{100}{\pi} \exp(-25|x|^2), & x \neq 0. \end{cases}$$

The initial data u_0 is taken to be such that its value at each lattice site is a randomly generated number between -1 (black) and 1 (white). As we can see in Figure 4.17, in this case the solution through u_0 coarsens to a monotonic equilibrium, also represented in Figure 4.18.

Experiment 4. Let us take the initial data

$$u_0(x) = 0.01 \sin(2\pi x), \quad x \in (0, 1).$$

Since $M = 0$, the homogeneous state in this case is $u \equiv 0$. We take $N = 100$, $\gamma = 1$, $\varepsilon = 0.8$ and J as in Section 3.7.2. The time evolution of the solution to (4.7.2) through u_0 is represented in Figure 4.19. One can observe the development of small wavelength spatial oscillations with large amplitude. At time $t = 2 \times 10^4$ the

solution appears to be periodic. The solution then coarsens to a final state which, unlike the equilibrium state of the Cahn-Hilliard equation, is not monotonic (it is only partially coarsened).

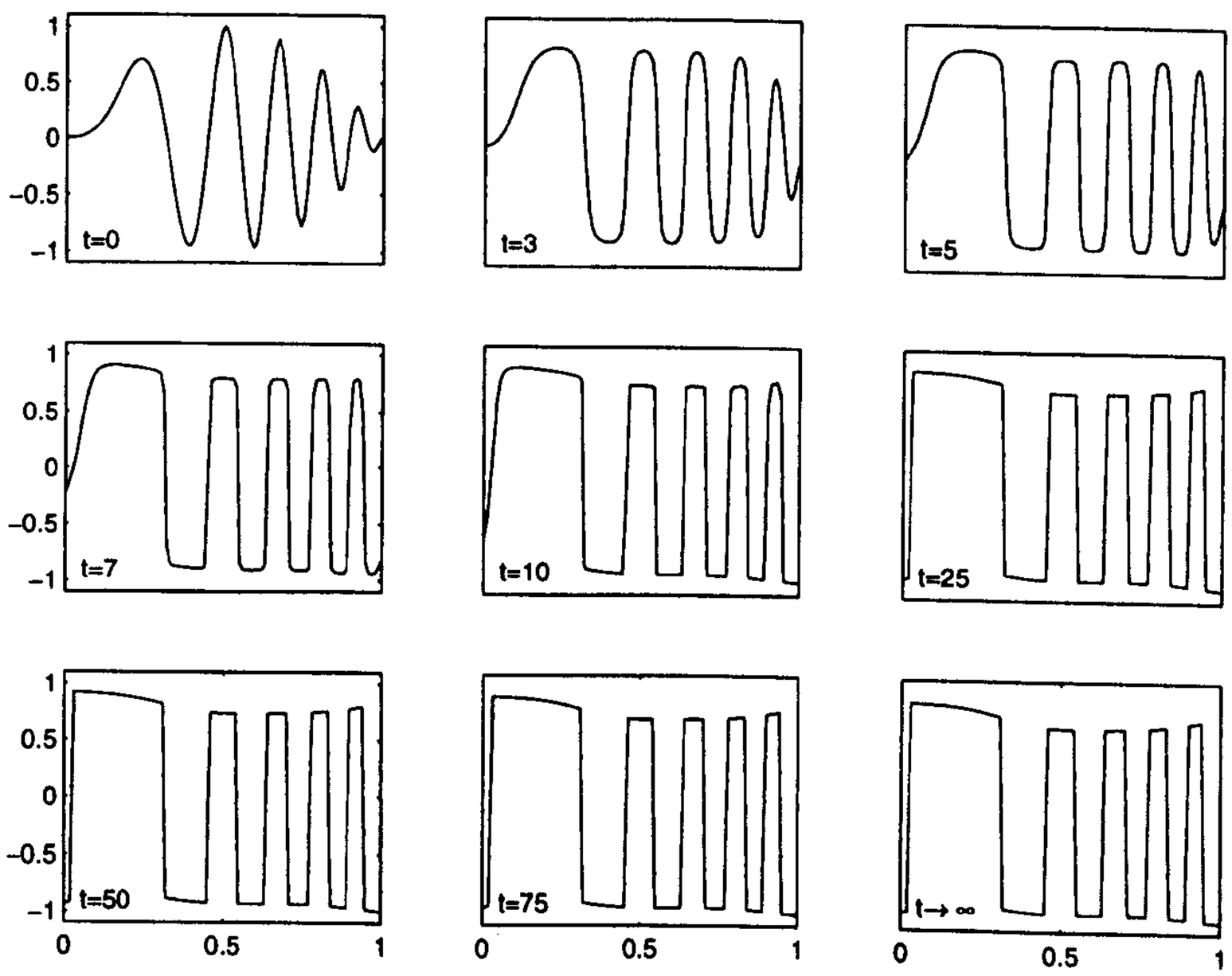

Figure 4.3: Time evolution of the solution of (4.7.1) with $\varepsilon = 1$ and $\gamma = 0.25$.

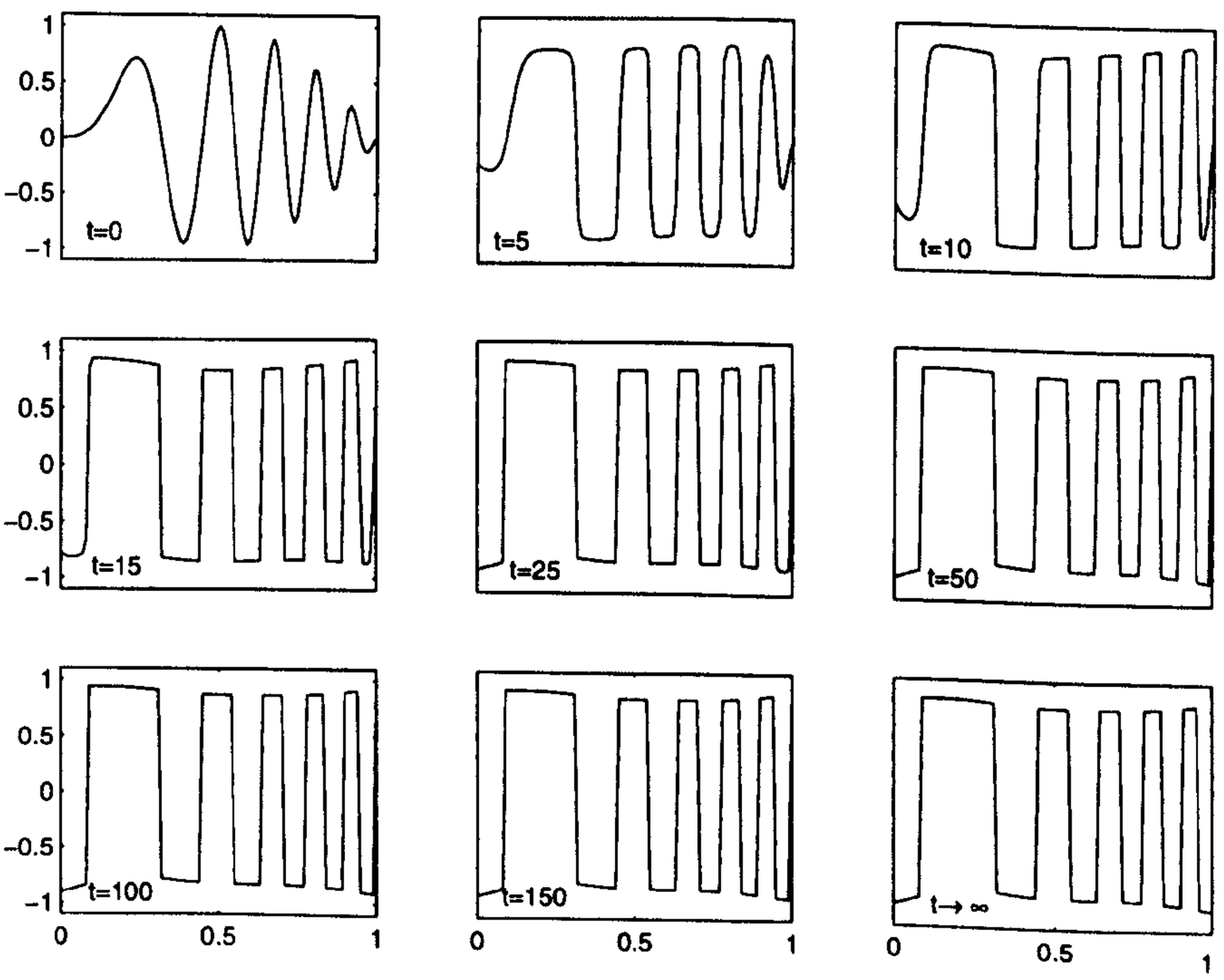

Figure 4.4: Time evolution of the solution of (4.7.2) with $\varepsilon = 1$ and $\gamma = 0.25$.

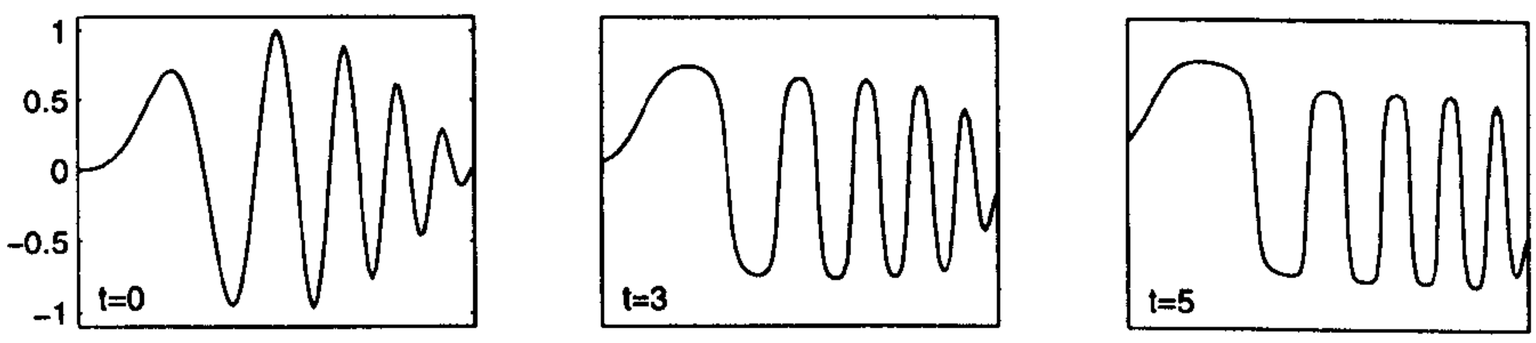

Figure 4.5: Time evolution of the solution of (4.7.1) with $\varepsilon = 1$ and $\gamma = 0.5$.

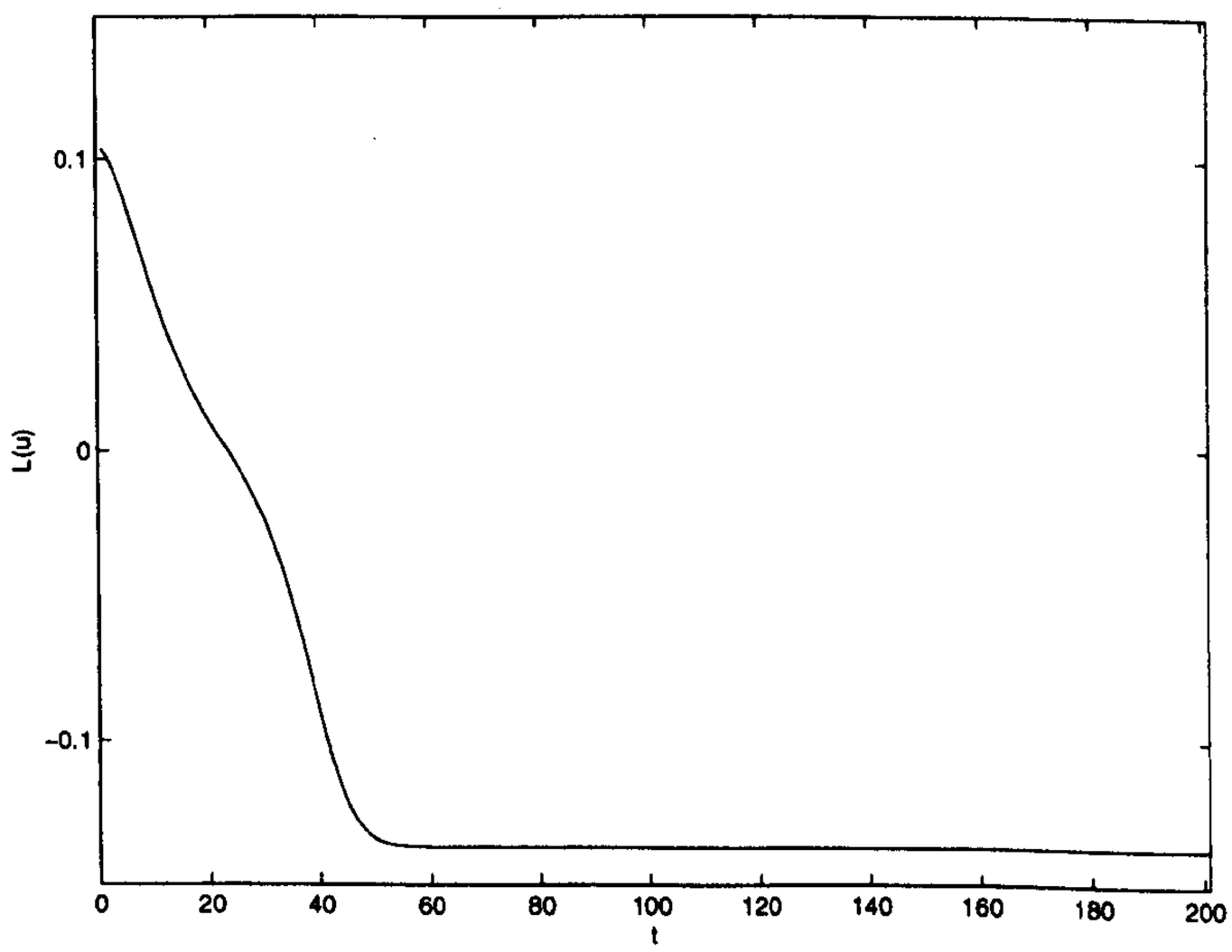

Figure 4.6: The Lyapunov function against time calculated using the solutions of (4.7.1), for $\gamma = 0.5$, $\varepsilon = 1$.

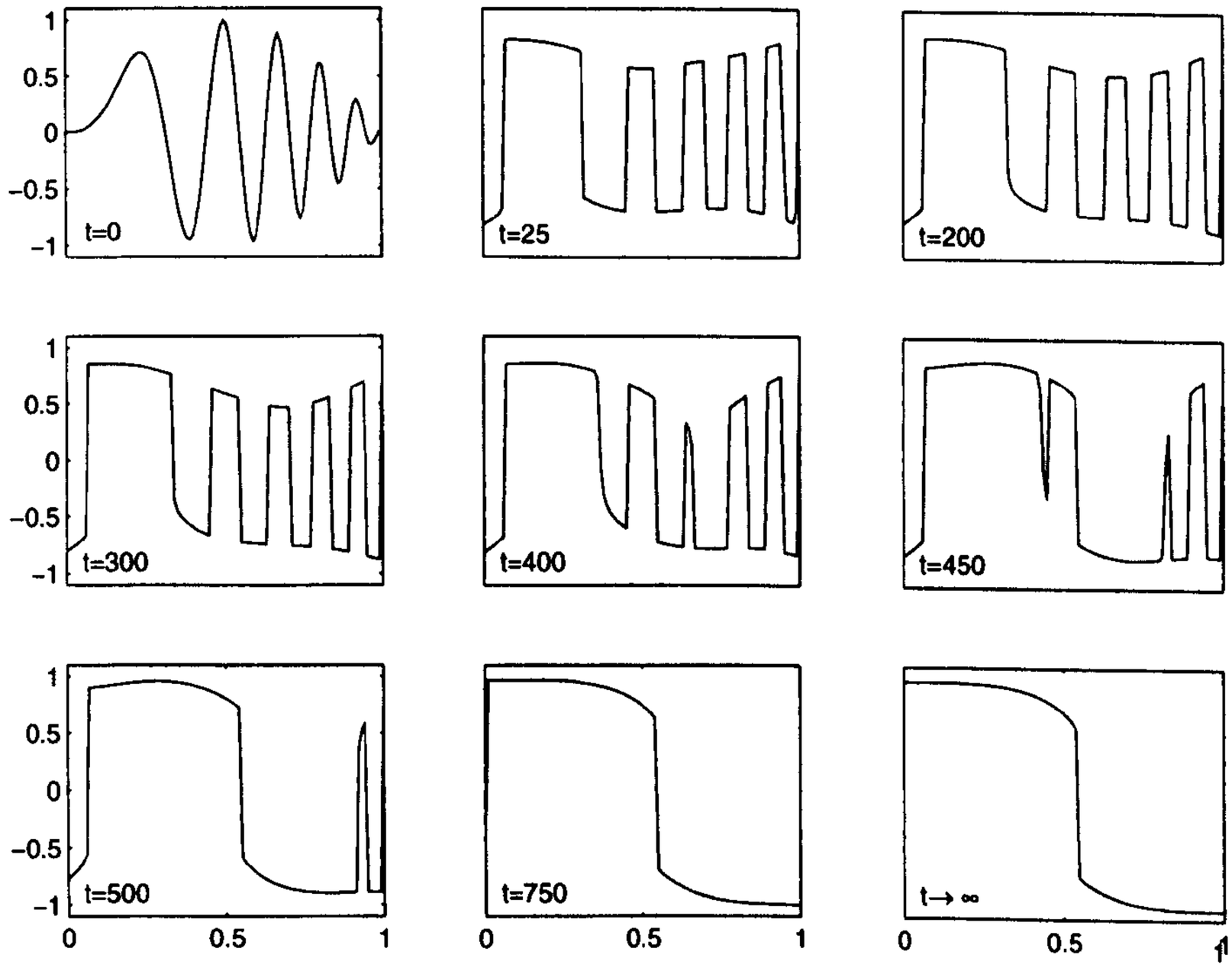

Figure 4.7: Time evolution of the solution of (4.7.2) with $\varepsilon = 1$ and $\gamma = 0.5$.

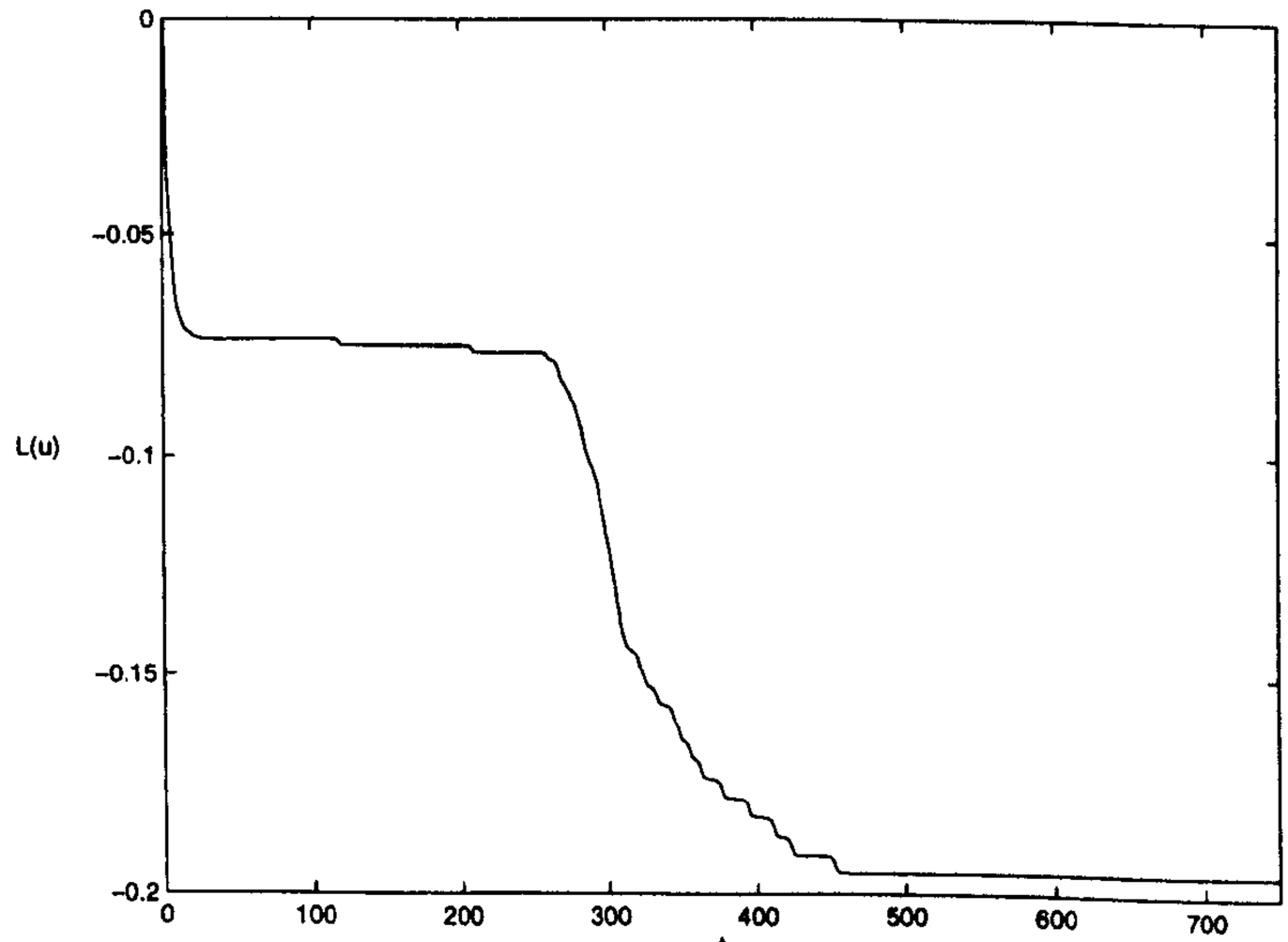

Figure 4.8: The Lyapunov function against time calculated using the solutions of (4.7.2), for $\gamma = 0.5$, $\varepsilon = 1$.

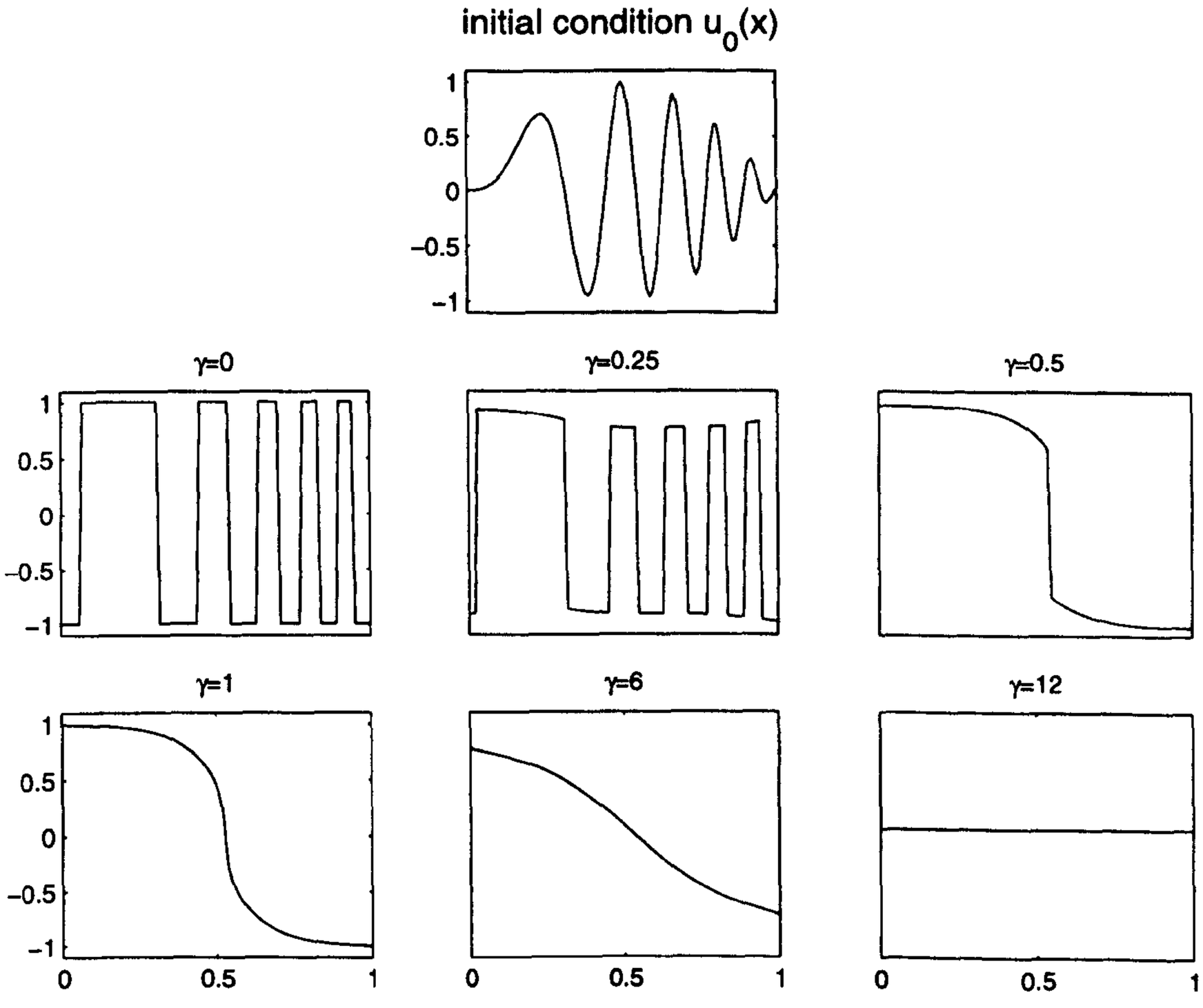

Figure 4.9: Initial data and equilibrium solutions of (4.7.1) for different values of γ and $\varepsilon = 1$.

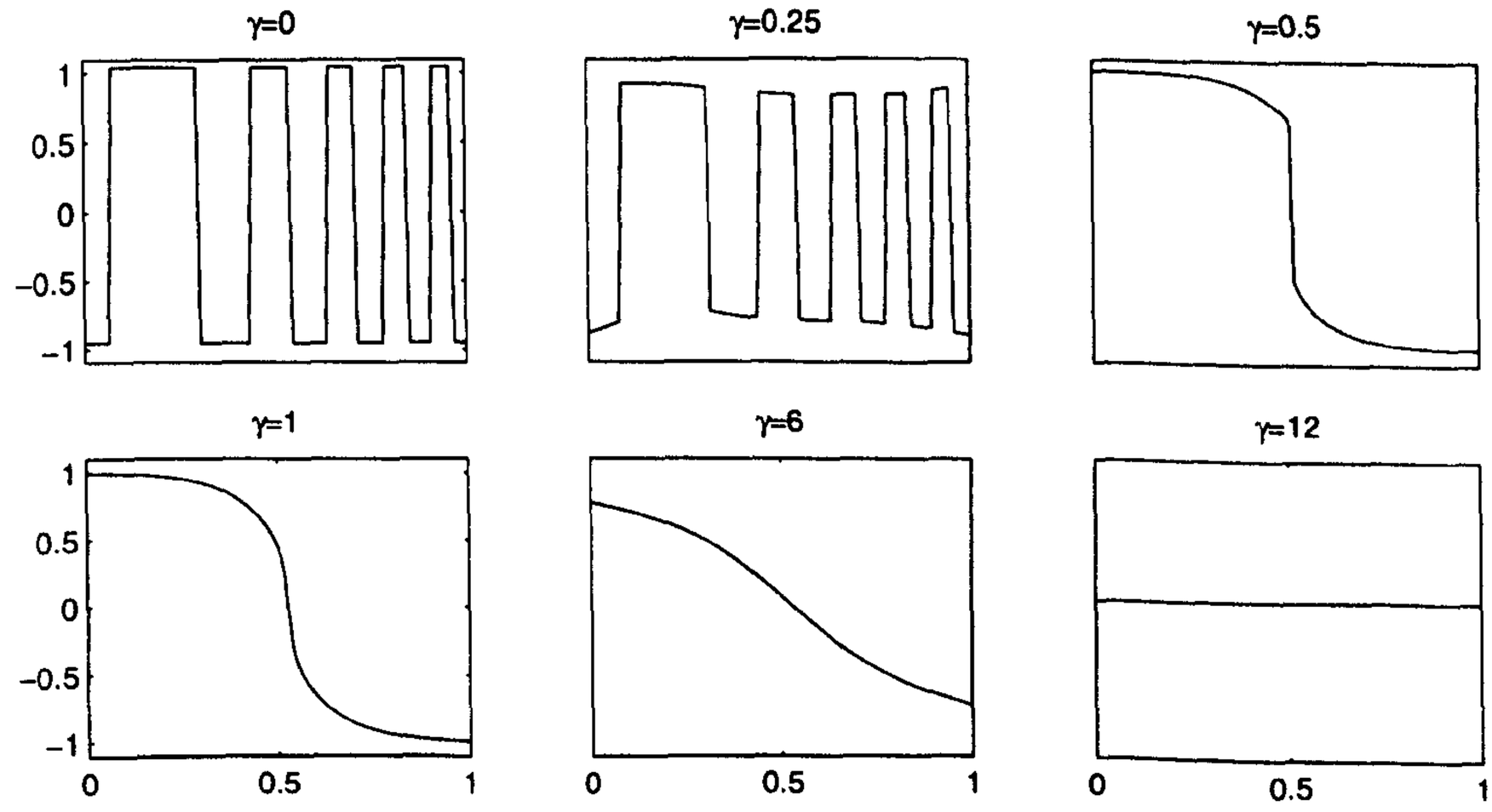

Figure 4.10: Equilibrium solutions of (4.7.2) for different values of γ and $\varepsilon = 1$.

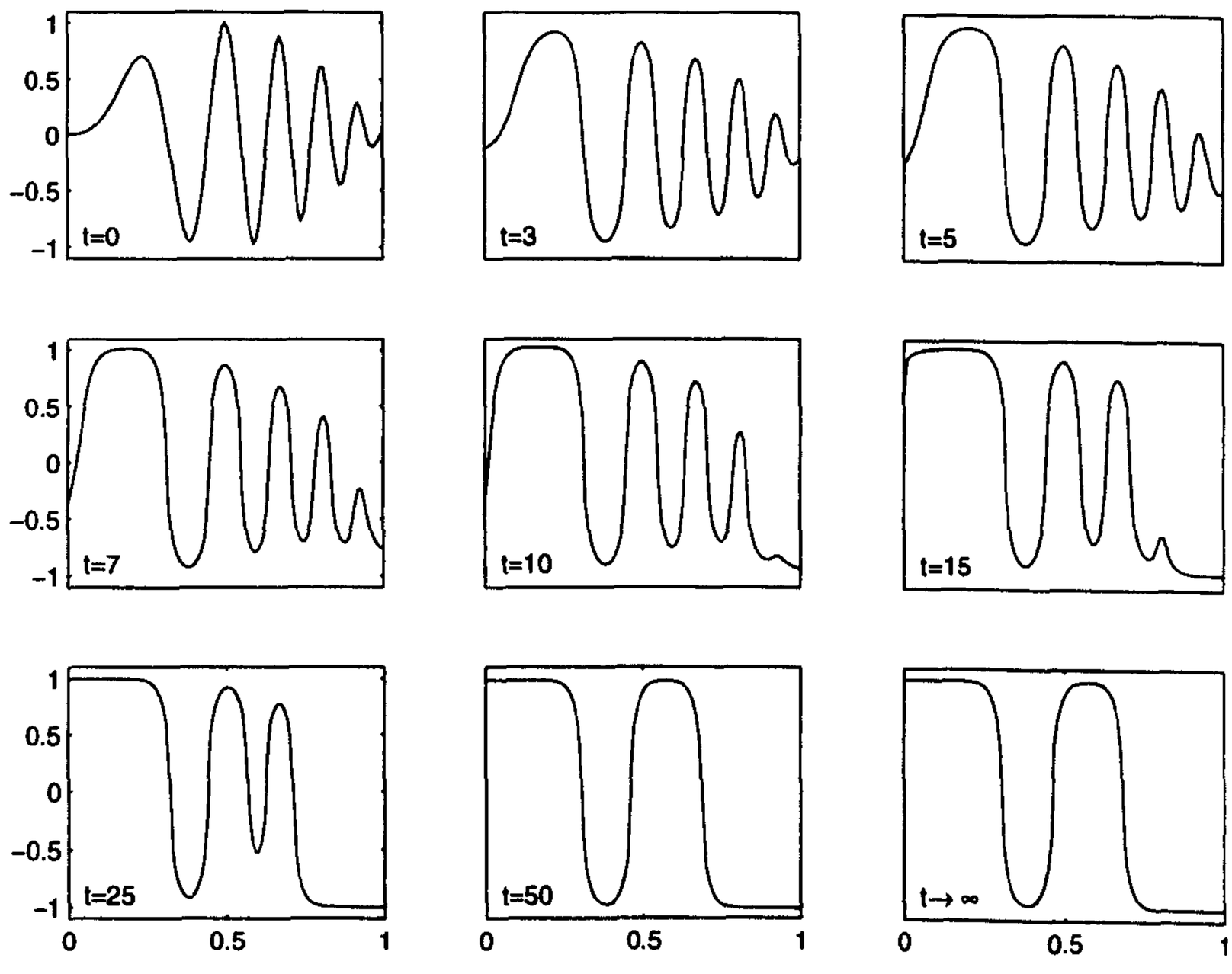

Figure 4.11: Time evolution of the solution of (4.7.1) with $\gamma = 1$ and $\varepsilon = 0.2$.

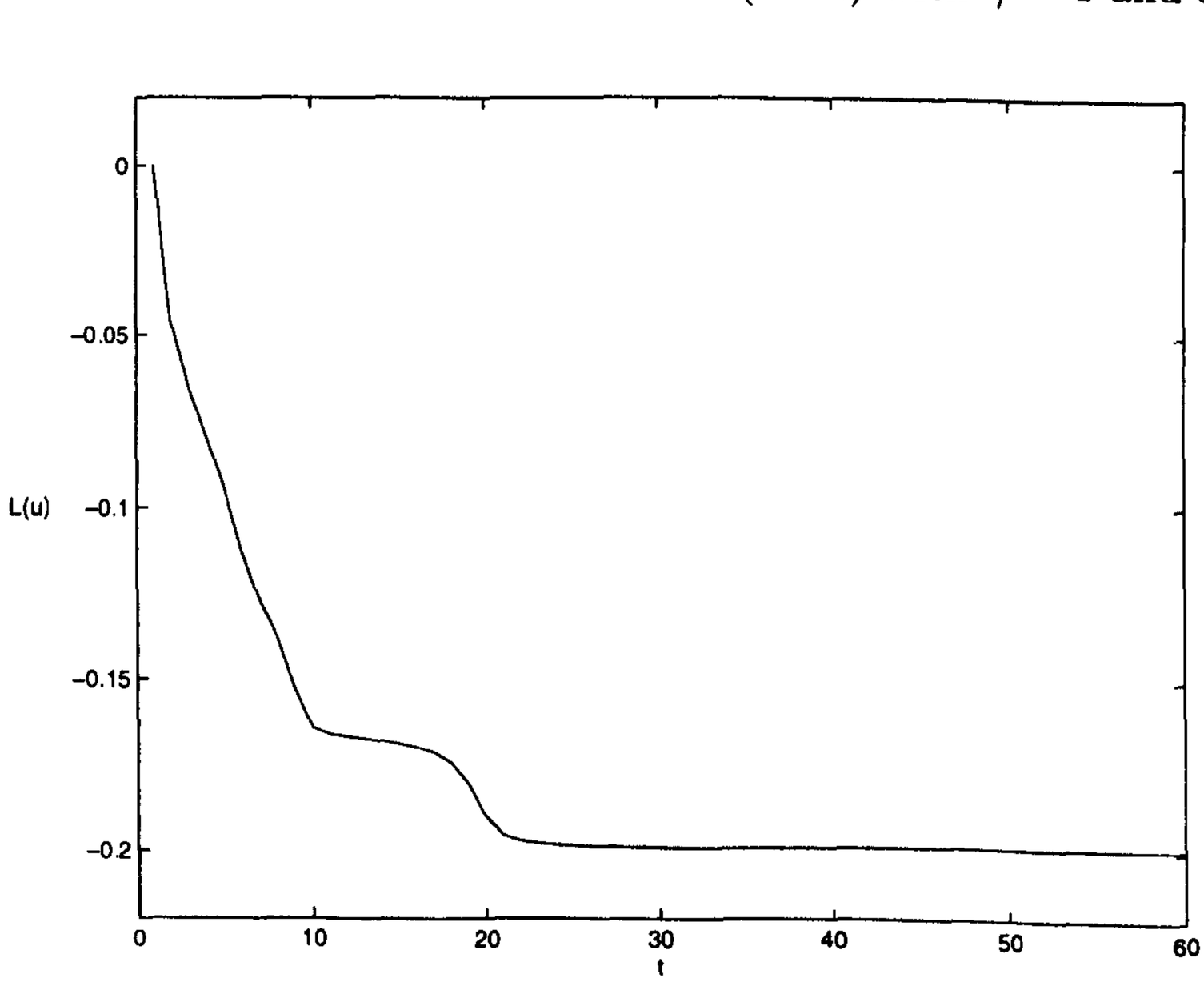

Figure 4.12: The Lyapunov function against time, calculated using the solutions of (4.7.1), for $\gamma = 1$, $\varepsilon = 0.2$.

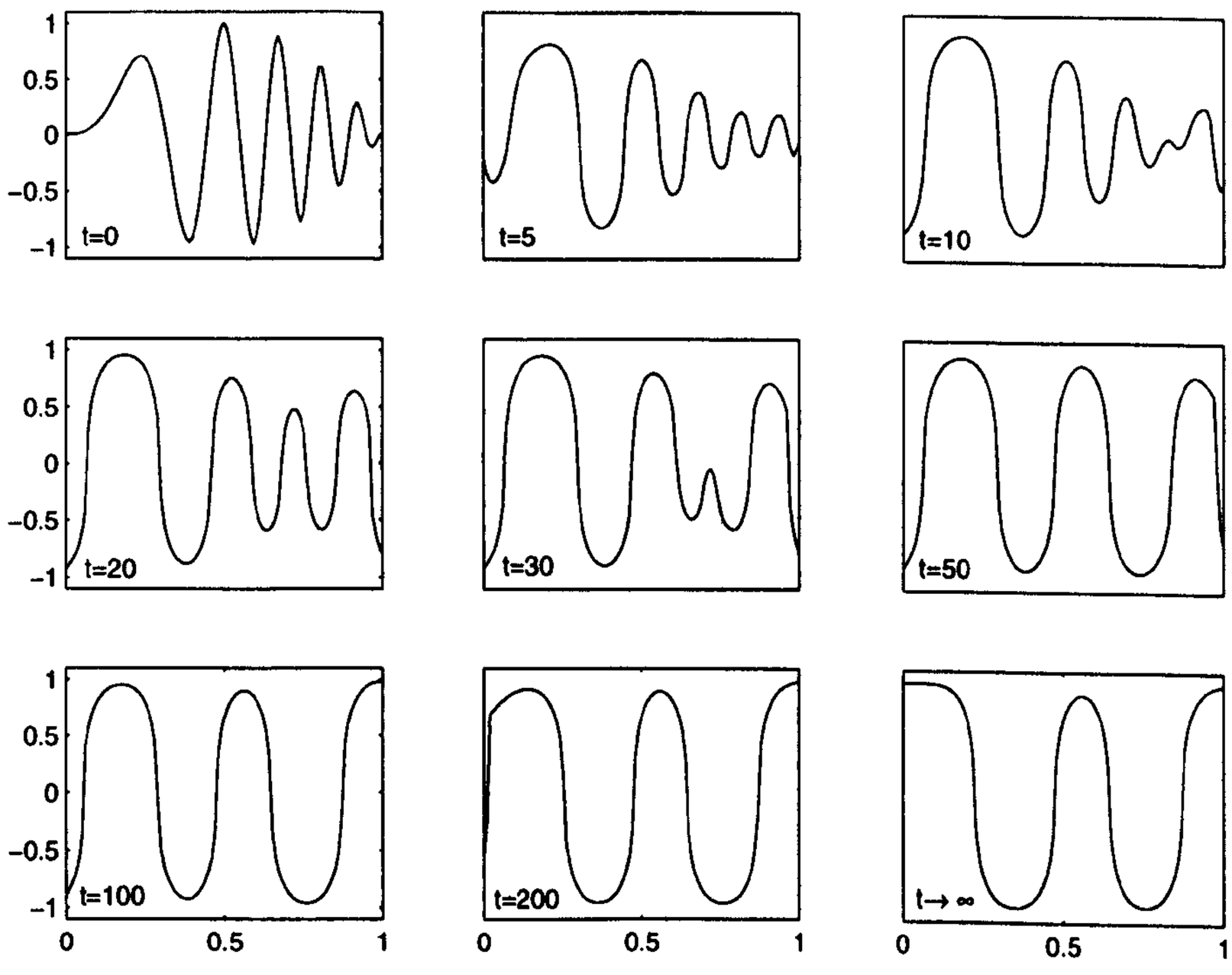

Figure 4.13: Time evolution of the solution of (4.7.2) with $\gamma = 1$ and $\varepsilon = 0.3$.

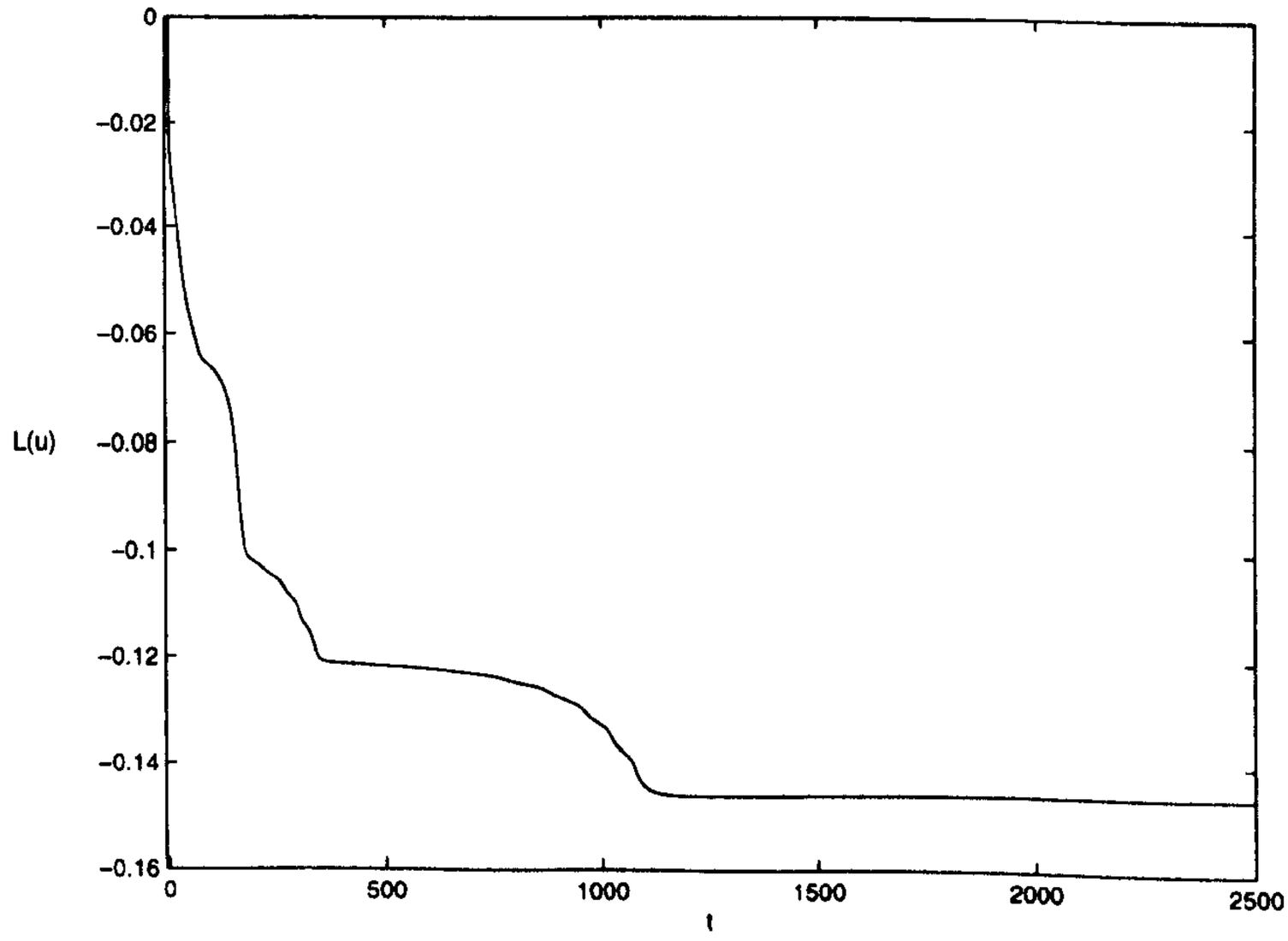

Figure 4.14: The Lyapunov function against time, calculated using the solutions of (4.7.2), for $\gamma = 1$, $\varepsilon = 0.3$.

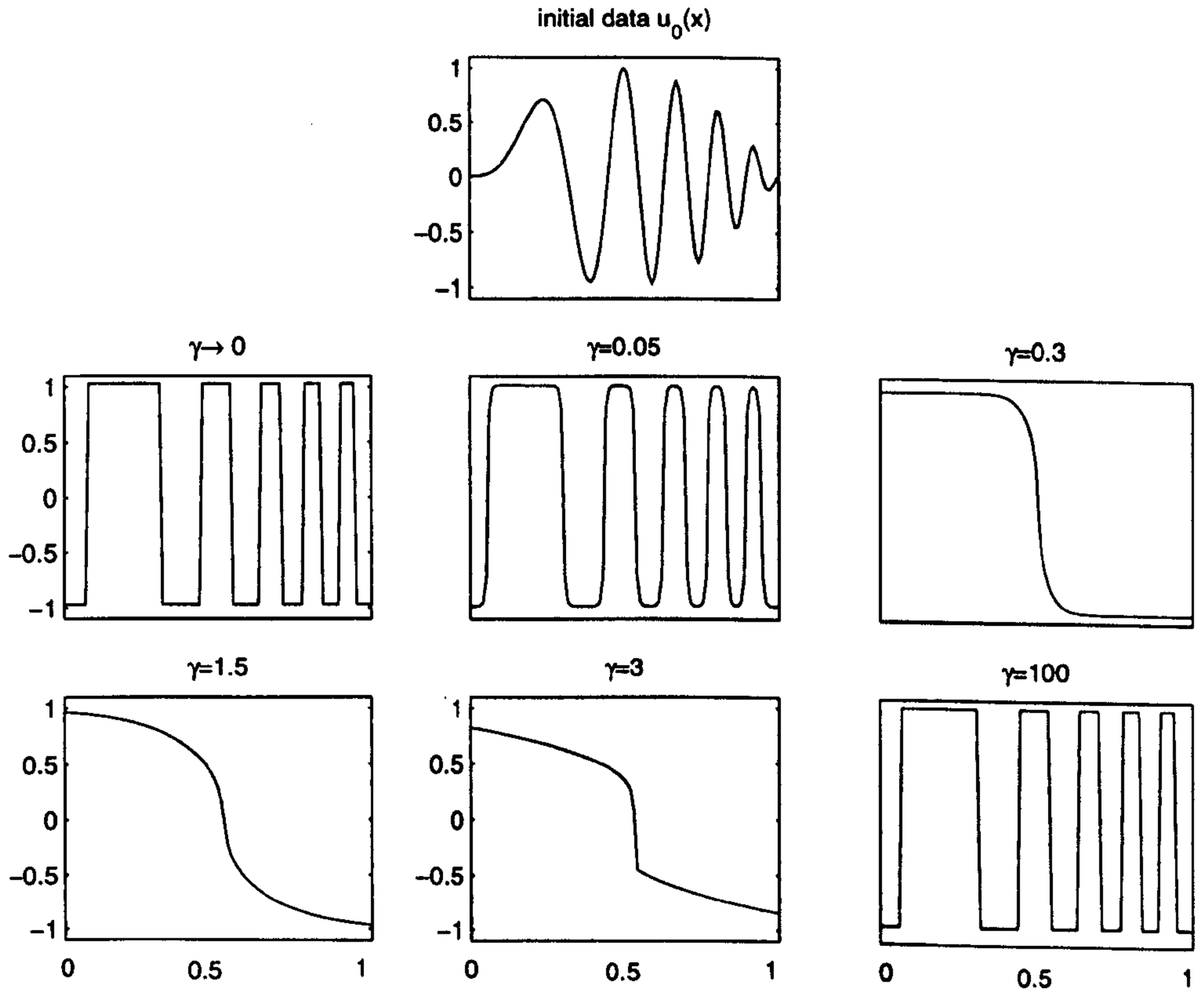

Figure 4.15: Initial data and equilibrium solutions of (4.7.1) for different values of ε and $\gamma = 1$.

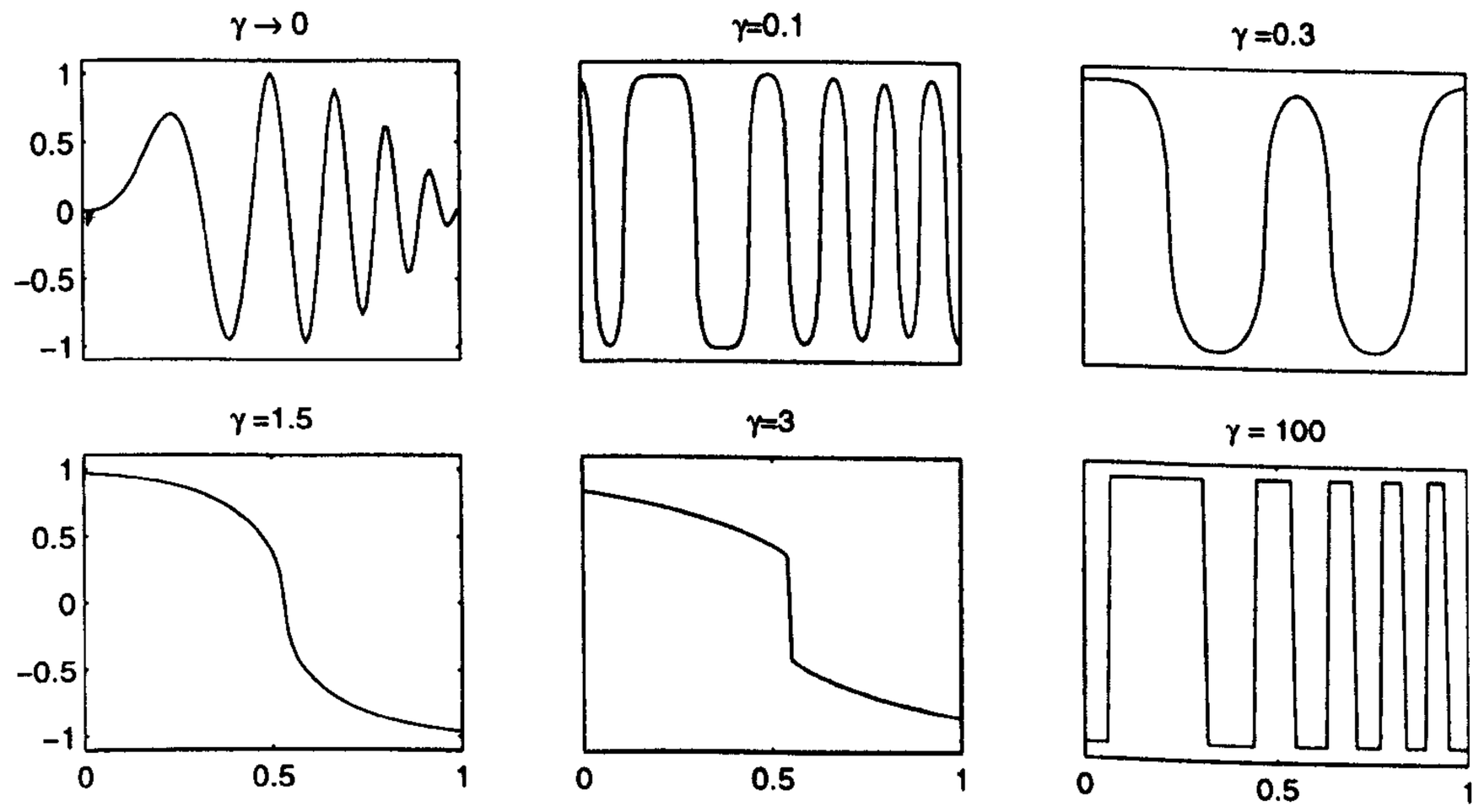

Figure 4.16: Equilibrium solutions of (4.7.2) for different values of ε and $\gamma = 1$.

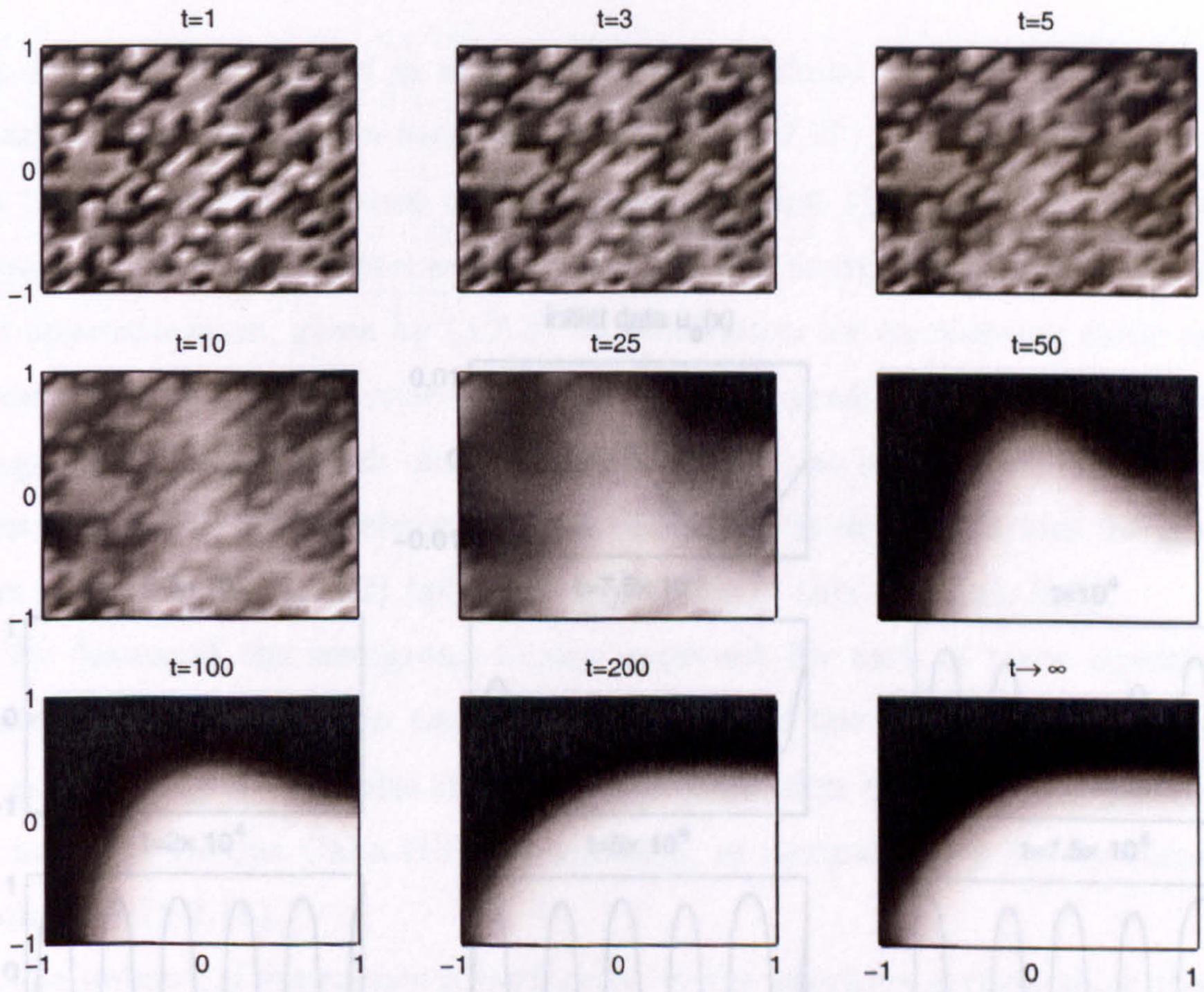

Figure 4.17: Time evolution of the solutions of (4.7.1) with $\epsilon = 1$ and $\gamma = 2$.

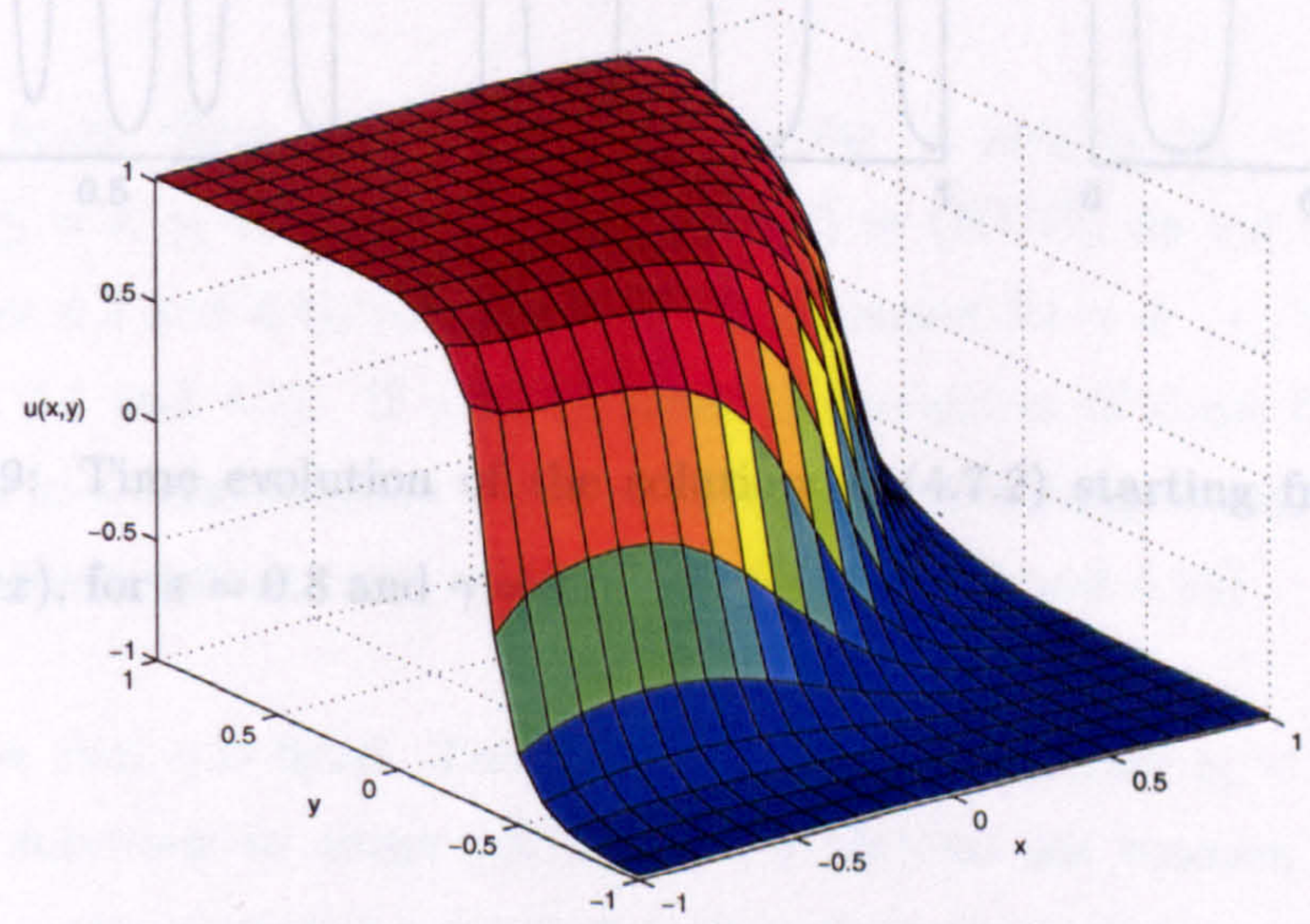

Figure 4.18: Equilibrium solution of (4.7.1) with $\varepsilon = 1$ and $\gamma = 2$.

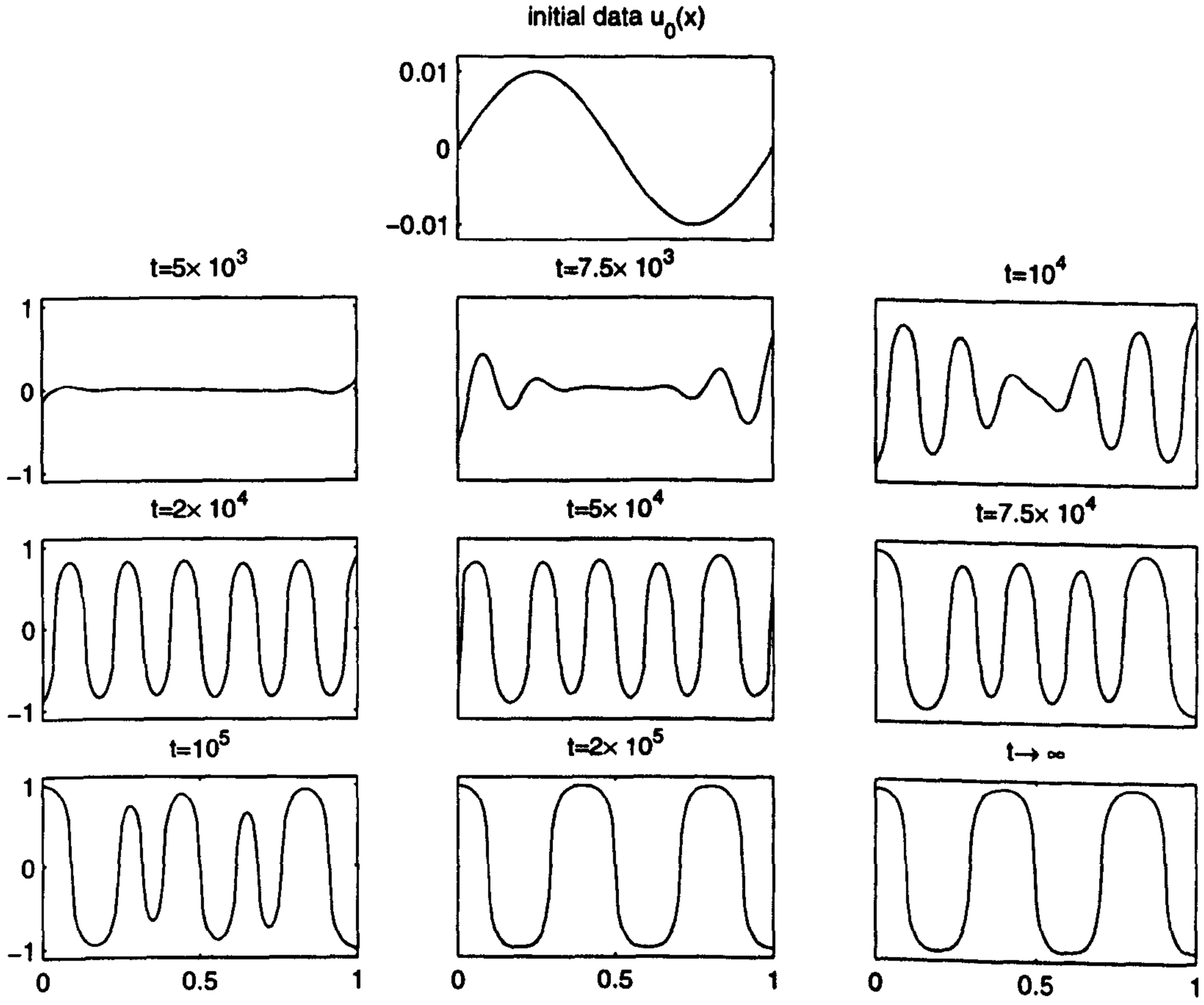

Figure 4.19: Time evolution of the solution of (4.7.2) starting from $u_0(x) = 0.01\sin(2\pi x)$, for $\varepsilon = 0.8$ and $\gamma = 1$.

4.8 Conclusions

The equations introduced in this chapter are nonlocal versions of the following equations: the Rubinstein-Sternberg equation (2.2.20), the Cahn-Hilliard equation (2.2.19) and the viscous Cahn-Hilliard equation (2.2.15). They are derived as gradient flows of the exact expression of the free energy functional in the mean-field approximation, given by (3.2.3). A motivation for considering these models rather than the classical ones is the fact that the gradient expansion of the free energy (3.2.3) (from which one can obtain (2.2.12) as the first-order truncation) is not valid when the wavelength of microstructure is very small, and the gradient flows derived from (2.2.12) fail to be applicable in this case (see [66]).

We discussed the semigroup theory approach for each of these equations in appropriate Hilbert spaces and some properties of the steady state solutions in the case $J(\cdot) \geq 0$. We also discussed the dispersion relation corresponding to the nonlocal viscous Cahn-Hilliard equation, in comparison with the dispersion relation for (2.2.15).

The numerical experiments performed in the previous section show the non-coarsening property of solutions of (NRS) and (NCH) for certain values of the parameters ϵ and γ. This property is not common to their local analogues. Based on these experiments, we can conjecture the following:

1. For ϵ fixed, there are two values of γ, say γ_1 and γ_2 $(\gamma_1 < \gamma_2)$, so that for any $0 \leq \gamma < \gamma_1$ solutions to either (NRS) or (NCH) do not coarsen at all (see Figures 4.3 and 4.4), and they partially coarsen for $\gamma \in (\gamma_1, \gamma_2)$ (as shown in Figures 4.5 and 4.7). If $\gamma > \gamma_2$, then the solutions of these two equations do coarsen to a final solution which is monotone. For large enough γ this final solution is the constant mass solution (see Figures 4.9 and 4.10).

2. Suppose that γ is fixed. There exist four values of ϵ, say $\epsilon_1 < \epsilon_2 < \epsilon_3 < \epsilon_4$, such that solutions to either (NRS) or (NCH) do not coarsen at all if $\epsilon \in (0, \epsilon_1) \bigcup (\epsilon_4, \infty)$, a partial coarsening takes place for $\epsilon \in (\epsilon_1, \epsilon_2) \bigcup (\epsilon_2, \epsilon_3)$ (as shown in Figures 4.11 and 4.13). For $\epsilon \in (\epsilon_2, \epsilon_3)$ the solutions do coarsen to a

monotonic solution (see Figures 4.15 and 4.16).

As in the case of the Cahn-Hilliard equation, one can observe numerically (see Figure 4.19) that most solutions of (NCH) starting in a small neighbourhood of the homogeneous solution undergo spinodal decomposition. The difference is that, after the fine-grained decomposition, solutions will partially coarsen, and the final solution is not necessarily monotonic.

Chapter 5

Models from Statistical Mechanics

5.1 Introduction

Statistical Mechanics provides a bridge between the macroscopic realm of classical thermodynamics and the microscopic realm of atoms and molecules. One can calculate the thermodynamic properties of a system by applying Statistical Mechanics principles. Of particular interest for materials science is the ability to calculate free energies associated with a variety of processes, such as ferromagnetism and phase separation in binary mixtures.

Statistical Mechanics has provided a good source of nonlocal evolution models for phase transitions. As we have seen in Chapter 1, the Ising model provides a useful description for physical systems in which certain variables of the system can take two distinct discrete values.

The models (1.2.9) and (1.2.10) presented in Section 1.2.3 are deterministic equations for the expectation of site occupation as a function of time. It was shown [86] that each of these equations has a Lyapunov function, which can be interpreted as a free energy, even though the expression of the Lyapunov function in the Kawasaki dynamics case (see (1.2.14)) is not quite the free energy of the

system in the mean-field approximation.

Until recent years the phase separation phenomenon in binary alloys was mostly studied using the direct-exchange between neighbouring atoms (see, for example, [26], [27]) despite the fact that this mechanism is unrealistic. However, in metallic alloys the atoms interchange places rather via a vacancy mechanism, which is explained in the beginning of the next section.

The work of Yaldram and Binder [101] is the first one in which a model of a binary alloy containing a small number of vacancies was considered. In this paper the diffusion process takes place only via the vacancy mechanism rather than by direct exchange. They performed Monte Carlo simulations for a binary alloy containing two types of atoms and a small number of vacancies, and found the same type of patterns for domain structure as in the case of the direct exchange model. It was concluded that the choice of diffusion mechanism (direct exchange or vacancy diffusion) is of minor importance for the phase separation process in a binary mixture.

Comparative Monte Carlo simulations for the Kawasaki model on one side and a vacancy mediated model on the other were also performed in [49] (see also [51] and the comments in [50] and [52]), where there was considered only a vacant site, the other sites being occupied by A and B atoms. They observed some differences between these models in the very early stages, which are due to the fact that the vacancy acts locally in the beginning, but the patterns seemed to be extremely similar in the later stages. The surprise came from the fact that, in terms of computing time, the process went up to 30 times faster with vacancy diffusion.

Representations of the diffusion process in real alloys via the vacancy mechanism have been also considered in [98] and [99] for the NCOP case. It was found that the vacancies prefer to stay in the disordered regions, and they concluded that the process cannot be described only by a system of two Allen-Cahn equations. A third equation describing the dependence of the vacancy diffusion on the local order parameter must also be considered.

Our purpose in this chapter is to study the mean-field dynamics of a binary mixture where the interchange of atoms is mediated by vacancies. To this end we

shall use and adapt the method developed by Penrose and presented in Section 1.2.3. The dynamics can be described by using two equations, which we derive in the next section. We show that the new system of equations admits a Lyapunov functional, which can be useful in deducing mathematical properties of the solutions of the system. We also do some numerics and compare them with those of the mean-field equations derived using Kawasaki dynamics.

5.2 Ising model with vacancy-driven dynamics

Let us consider a lattice Λ which has a small (the meaning of this term will be specified later) number of empty sites, the other sites being populated by atoms of two types, A or B. At a given moment of time, t, each lattice site k can be occupied by either an A-atom with probability $P_A(k;\, t)$, or a B-atom with probability $P_B(k;\, t)$, or stay vacant with probability $P_V(k;\, t)$. Clearly, these probabilities satisfy the following normalization condition

$$P_A(k;\, t) + P_B(k;\, t) + P_V(k;\, t) = 1, \quad \text{for all } k \in \Lambda, \quad t > 0.$$

To each lattice site k we assign three occupation variables (*spins*): s_k, r_k and q_k, such that $s_k = 1$ if the site k is taken by an A-atom and $s_k = 0$ otherwise, $r_k = 1$ if the site k is taken by a B-atom and $r_k = 0$ otherwise, $q_k = 1$ if the site k is vacant and $q_k = 0$ otherwise. Obviously, we have

$$s_k + r_k + q_k = 1, \quad \text{for all } k \in \Lambda,$$

which means that the system has two degrees of freedom, and thus two evolution equations are necessary to describe the occupancy of each site in time. We denote by $N(k)$ the set of all nearest neighbour sites of the lattice site k and consider the configuration (s, r), where $s = \{s_m, m \in \Lambda\}$, $r = \{r_n, n \in \Lambda\}$. By a *configuration* we understand a specification of the values of spin components, which corresponds to a distribution of atoms on the lattice sites. If only the nearest neighbour interactions are taken into account, then the energy of the configuration (s, r) is

given by:

$$W(s,r) = -\frac{1}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)} J_{kl}(s_k - r_k)(s_l - r_l), \tag{5.2.1}$$

where J_{kl} is the Ising interaction between sites k and l, which is assumed throughout to be nonnegative. As we can see, $W(s,r)$ decreases if $A-A$ and $B-B$ bonds are created and increases for $A-B$ and $B-A$ bonds. This means that an A-atom (B-atom) dislikes nearest neighbour B-atoms (A-atoms) and prefers having nearest neighbour also an A-atom (B-atom, respectively), but it does not matter energetically whether its nearest neighbour is a vacancy.

The system is considered to be initially at a high temperature, which is then decreased below a critical point where the structure may become unstable. We assume here the mechanism of diffusion via the interchange of atoms with vacancies: an A-atom or a B-atom may jump to a vacant nearest neighbour site with a certain transition probability (which depends upon the type of the atom and the neighbour lattice sites involved); no direct $A-B$ interchanges are permitted. After a short transient we would expect to see the separation of the system into A-rich and B-rich regions.

We now want to derive two equations which will describe the evolution of the system in time. Let us consider a pair of interchange sites at (k, l), with $k \in \Lambda$ and l a nearest-neighbouring site. If we have an A-atom at k and a vacancy at l, we denote by $\omega_{kl}(s)$ the probability per unit time that the spins of the s-configuration at the two sites will change places (this represents the rate at which the A-atom jumps to the vacant site l), and by $\omega_{kl}(s^{kl})$ the probability per unit time that the spins at sites k and l of the configuration s^{kl} will change places, where s^{kl} is the configuration obtained from s by interchanging s_k and s_l (this probability is the rate at which an A-atom appears at site k by jumping in from the vacant nearest neighbour site l). Mathematically, we define the components of the configuration s^{kl} in the following way:

$$(s^{kl})_p = \begin{cases} s_p, & \text{if } p \neq k, l \\ s_k, & \text{if } p = l \\ s_l, & \text{if } p = k. \end{cases}$$

For each lattice site k we aim to find the evolution equations for the expected value of the spins s_k and q_k. To this end, we need to rewrite the energy (5.2.1) in terms of s and q -spins. For a configuration $(s,q) = \{(s_m, q_n);\ m \in \Lambda,\ n \in \Lambda\}$, the energy $W(s,\ r)$ can be written as:

$$W(s,q) = -\frac{1}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)} J_{kl}(2s_k + q_k - 1)(2s_l + q_l - 1). \tag{5.2.2}$$

An A-atom can appear at site k if this site is vacant and a nearest-neighbour A-atom jumps in there, and it can disappear when a nearest-neighbour site is empty. At a given moment of time, t, we denote by $P_{AV}(k,l;\ t)$ the probability of finding simultaneously an A-atom at site k and a vacancy at site l, and by $P_{VA}(k,l;\ t)$ the probability of finding simultaneously a vacancy at position k and an A-atom at site l. Then the rate of change of the probability that the site k be occupied by an A-atom is given by:

$$\frac{d}{dt}P_A(k;\ t) = \sum_{l\in N(k)} \{P_{VA}(k,l;\ t)\,\omega_{kl}(s^{kl}) - P_{AV}(k,l;\ t)\,\omega_{kl}(s)\}. \tag{5.2.3}$$

Equations of this type are usually called *the master equations*. We can write a similar equation for the rate of change of $P_V(k;\ t)$, which involves joint probabilities of type $P_{VC}(k,\ l;\ t)$, where C is either an A-atom or an B-atom. We make here a simplifying assumption: we suppose that the number of vacancies in the system is very low, such that if a site is vacant, then all the nearest neighbour sites are not empty. In terms of probabilities, our assumption can be written as

$$P_{VC}(k,l;\ t) = P_V(k;\ t),\ \text{for all sites } k \text{ and } l. \tag{5.2.4}$$

With other words, (5.2.4) says that the conditional probability $P(C \in l|\, V \in k;\ t)$ is 1. The site k would become vacant if it has a vacant nearest neighbour site and the atom which is initially at k jumps in there with the probability $\omega_{kl}(q^{kl})$, and k would no longer be vacant when a nearest neighbour atom appears at site k with the rate $\omega_{kl}(q)$. We thus can write the law for the rate of change of $P_V(k;\ t)$:

$$\frac{d}{dt}P_V(k;\ t) = \sum_{l\in N(k)} \{P_V(l;\ t)\,\omega_{kl}(q^{kl}) - P_V(k;\ t)\,\omega_{kl}(q)\}. \tag{5.2.5}$$

A complete statistical description of this dynamical system model would consist of the knowledge of the probabilities $P_A(k;\, t)$, $P_B(k;\, t)$ and $P_V(k;\, t)$, for each $k \in \Lambda$, at any time t. This is, however, impossible to calculate in practice, because of the complexity of the equations in (5.2.3) and (5.2.5), but one can calculate instead the expectation values of the spins s_k, q_k and r_k.

Let us denote the expected value of a random variable by the symbol $\mathbf{E}$. Then

$$\mathbf{E}(s_k) = P_A(k;\, t), \quad \mathbf{E}(q_k) = P_V(k;\, t), \quad \text{for all } k \in \Lambda,$$

and we can write the equations (5.2.3) and (5.2.5) in terms of expected values. From the definitions of s_k and q_k, we get the following probability distributions:

$$s_l q_k \omega_{kl}(s^{kl}) : \begin{pmatrix} 0 & \omega_{kl}(s^{kl}) \\ 1 - P_{VA}(k,l;\, t) & P_{VA}(k,l;\, t) \end{pmatrix}$$

and similarly,

$$s_k q_l \omega_{kl}(s) : \begin{pmatrix} 0 & \omega_{kl}(s) \\ 1 - P_{AV}(k,l;\, t) & P_{AV}(k,l;\, t) \end{pmatrix}.$$

(The first row contains the values of the random variable, and below each value is written the probability that the variable take the specified value.) A simple calculation shows that

$$\mathbf{E}[(s_l q_k - s_k q_l)\omega_{kl}(s)] = P_{VA}(k,l;\, t)\, \omega_{kl}(s^{kl}) - P_{AV}(k,l;\, t)\, \omega_{kl}(s),$$

and thus, we can write (5.2.3) in the form

$$\frac{d}{dt}\mathbf{E}(s_k) = \sum_{l \in N(k)} \mathbf{E}[(s_l q_k - s_k q_l)\, \omega_{kl}(s)]. \tag{5.2.6}$$

In a similar manner, from (5.2.5) we get

$$\frac{d}{dt}\mathbf{E}(q_k) = \sum_{l \in N(k)} \mathbf{E}[q_l - q_k)\, \omega_{kl}(q)]. \tag{5.2.7}$$

It only remains now to specify the transition probabilities $\omega_{kl}(s)$ and $\omega_{kl}(q)$. Following [54] (see also [92]), if the equilibrium of the system is reached at some

temperature T, then each of these rates is inversely proportional to the Maxwell-Boltzmann factor $e^{-W(s,q)/\kappa T}$, where the parameter κ is the Boltzmann's constant and T is the temperature. We shall denote $\frac{1}{\kappa T}$ by β. These rates should thus satisfy the *detailed balance conditions*:

$$\omega_{kl}(s)e^{-\beta W(s,q)} = \omega_{kl}(s^{kl})e^{-\beta W(s^{kl},q)} \tag{5.2.8}$$

and, respectively,

$$\omega_{kl}(q)e^{-\beta W(s,q)} = \omega_{kl}(q^{kl})e^{-\beta W(s,q^{kl})}. \tag{5.2.9}$$

A convenient choice of the transition rates which satisfy the detailed balance is the Glauber's hyperbolic tangent rule ([54], [86], [92]). For $\omega(s)$ the rule is:

$$\omega(s) = \frac{1}{2}\{1 - \tanh[\frac{1}{2}\beta\delta W(s)]\}, \tag{5.2.10}$$

and for $\omega(q)$,

$$\omega(q) = \frac{1}{2}\{1 - \tanh[\frac{1}{2}\beta\delta W(q)]\}, \tag{5.2.11}$$

where $\delta W(s)$ is the difference between the internal energy after and before the swap of the s-spins at positions k and l. In our case ω stands for ω_{kl} and

$$\delta W(s) = W(s^{kl}, q) - W(s, q),$$

$$\delta W(q) = W(s, q^{kl}) - W(s, q).$$

Let us now calculate $\delta W(s)$. We have:

$$\begin{aligned} W(s,q) &= -\frac{1}{2}\sum_{m\in\Lambda}\sum_{n\in N(k)} J_{mn}(2s_m + q_m - 1)(2s_n + q_n - 1) \\ &= -\frac{1}{2}\sum_{m\neq k,l}\sum_{\substack{n\neq k,l \\ n\in N(l)}} J_{mn}(2s_m + q_m - 1)(2s_n + q_n - 1) \\ &- \sum_{n\neq k} J_{ln}(2s_l + q_l - 1)(2s_n + q_n - 1) \\ &- \sum_{\substack{m\in N(k) \\ m\neq l}} J_{km}(2s_k + q_k - 1)(2s_m + q_m - 1) \\ &- J_{kl}(2s_k + q_k - 1)(2s_l + q_l - 1), \end{aligned}$$

and

$$W(s^{kl},q) = -\frac{1}{2}\sum_{m\neq k,l}\sum_{n\neq k,l} J_{mn}(2s_m+q_m-1)(2s_n+q_n-1)$$
$$-\sum_{\substack{n\in N(l)\\ n\neq k}} J_{ln}(2s_k+q_l-1)(2s_n+q_n-1)$$
$$-\sum_{\substack{m\in N(k)\\ m\neq l}} J_{km}(2s_l+q_k-1)(2s_m+q_m-1)$$
$$-J_{kl}(2s_l+q_k-1)(2s_k+q_l-1),$$

where $n \in N(m)$ in the double sums of the above expressions. We thus get:

$$\delta W(s) =$$
$$= 2(s_k-s_l)[\sum_{m\neq l}^{m\in N(k)} J_{km}(2s_m+q_m-1) - \sum_{n\neq k}^{n\in N(l)} J_{ln}(2s_n+q_n-1) + J_{kl}(q_l-q_k)]$$
$$= 2(s_k-s_l)[\sum_{m\in N(k)} J_{km}(2s_m+q_m-1) - \sum_{n\in N(l)} J_{ln}(2s_n+q_n-1) + 2J_{kl}(s_k-s_l)]$$

In order to find the corresponding expression for $\delta W(q)$, we need $W(s,q^{kl})$. This is given by

$$W(s,q^{kl}) = -\frac{1}{2}\sum_{m\neq k,l}\sum_{n\neq k,l} J_{mn}(2s_m+q_m-1)(2s_n+q_n-1)$$
$$-\sum_{\substack{m\in N(k)\\ m\neq l}} J_{km}(2s_k+q_l-1)(2s_m+q_m-1)$$
$$-\sum_{\substack{n\in N(l)\\ n\neq k}} J_{ln}(2s_l+q_k-1)(2s_n+q_n-1)$$
$$-J_{kl}(2s_k+q_l-1)(2s_l+q_k-1).$$

Since $\delta W(q) = W(s,q^{kl}) - W(s,q)$, we have

$$\delta W(q) =$$
$$= (q_k-q_l)[\sum_{m\neq l}^{m\in N(k)} J_{km}(2s_m+q_m-1) - \sum_{n\neq k}^{n\in N(l)} J_{ln}(2s_n+q_n-1) + 2J_{kl}(s_l-s_k)]$$
$$= (q_k-q_l)[\sum_{m\in N(k)} J_{km}(2s_m+q_m-1) - \sum_{n\in N(l)} J_{ln}(2s_n+q_n-1) + J_{kl}(q_k-q_l)]$$

Let us define the following two quantities:

$$\gamma_k = \sum_{m \in N(k)} J_{km}(2s_m + q_m - 1) \qquad (\equiv \sum_{m \in N(k)} J_{km}(s_m - r_m))$$

and

$$\gamma_l = \sum_{n \in N(l)} J_{ln}(2s_n + q_n - 1) \qquad (\equiv \sum_{n \in N(l)} J_{ln}(s_n - r_n)).$$

By substituting the expression of $\delta W(s)$ into (5.2.10), and then of $\delta W(q)$ into (5.2.11), we get the expressions for the transition rates $\omega_{kl}(s)$ and $\omega_{kl}(q)$, respectively. These are:

$$\omega_{kl}(s) = \frac{1}{2}\{1 - \tanh[\beta(s_k - s_l)(\gamma_k - \gamma_l + 2J_{kl}(s_k - s_l))]\} \tag{5.2.12}$$

and, respectively,

$$\omega_{kl}(q) = \frac{1}{2}\{1 - \tanh[\frac{\beta}{2}(q_k - q_l)(\gamma_k - \gamma_l + J_{kl}(q_k - q_l))]\}. \tag{5.2.13}$$

The above formulae are valid when k and l are nearest neighbour sites only. If this is not the case, we take $\omega_{kl} = 0$. Substitution of (5.2.12) and (5.2.13) into the time evolution equations (5.2.6) and (5.2.7), respectively, gives us:

$$\frac{d}{dt}\mathbf{E}(s_k) = \frac{1}{2}\sum_{l \in N(k)} \mathbf{E}\{(s_l q_k - s_k q_l)[1 - \tanh(\beta(s_k - s_l)(\gamma_k - \gamma_l + 2J_{kl}(s_k - s_l)))]\}$$

$$\frac{d}{dt}\mathbf{E}(q_k) = \frac{1}{2}\sum_{l \in N(k)} \mathbf{E}\{(q_l - q_k)[1 - \tanh(\frac{\beta}{2}(q_k - q_l)(\gamma_k - \gamma_l + J_{kl}(q_k - q_l)))]\}.$$

Since $(s_k - s_l) \in \{-1, 0, 1\}$ and $(q_k - q_l) \in \{-1, 0, 1\}$, the above equations can be written as:

$$\frac{d}{dt}\mathbf{E}(s_k) = \frac{1}{2}\sum_{l \in N(k)} \mathbf{E}\{(s_l q_k - s_k q_l)[1 - (s_k - s_l)\tanh(\beta(\gamma_k - \gamma_l + 2J_{kl}(s_k - s_l)))]\}$$

$$\frac{d}{dt}\mathbf{E}(q_k) = \frac{1}{2}\sum_{l \in N(k)} \mathbf{E}\{(q_l - q_k)[1 - (q_k - q_l)\tanh(\frac{\beta}{2}(\gamma_k - \gamma_l + J_{kl}(q_k - q_l)))]\}.$$

For each lattice site k we have $s_k^2 = s_k$, $q_k^2 = q_k$ and $s_k q_k = 0$. If $l \in N(k)$,

then one can easily check that

$$(s_l q_k - s_k q_l) = (s_l q_k + s_k q_l)(s_l - s_k)$$

$$(s_l q_k - s_k q_l)(s_l - s_k) = (s_l q_k + s_k q_l)(1 - s_l s_k)$$

and

$$q_l - q_k = (q_l + q_k)(q_l - q_k)$$

$$(q_l - q_k)^2 = (q_l + q_k)(1 - q_l q_k)$$

In order to find a convenient approximate model we use these identities to transform the last two equations into

$$\frac{d}{dt}\mathbf{E}(s_k) = \frac{1}{2}\sum_{l\in N(k)} \mathbf{E}\{(s_l q_k + s_k q_l)[(s_l - s_k) + \\ +(1 - s_l s_k)\tanh(\beta(\gamma_k - \gamma_l + 2J_{kl}(s_k - s_l)))]\} \qquad (5.2.14)$$

$$\frac{d}{dt}\mathbf{E}(q_k) = \frac{1}{2}\sum_{l\in N(k)} \mathbf{E}\{(q_l + q_k)[(q_l - q_k) - \\ -(1 - q_l q_k)\tanh(\frac{\beta}{2}(\gamma_k - \gamma_l + J_{kl}(q_k - q_l)))]\}. \qquad (5.2.15)$$

Up to this point the equations (5.2.14) and (5.2.15) give us the exact description of the kinetics of the dynamic Ising model with vacancy diffusion. Since these equations cannot be solved analytically, we would like to find some closed equations for $\mathbf{E}(s_k)$ and $\mathbf{E}(q_k)$. To this end, an approximation for the terms involving the expectation of the hyperbolic tangent is required. Due to the terms γ_l, in both equations the arguments of the hyperbolic tangent are sums of contributions from various parts of the system. We consider here a limiting case, when the interactions are very weak, so that we can assume that the fluctuations of these contributions about their mean values are independent. By applying a law of large numbers we get that fluctuations of each argument of the *tanh* function about its mean value will be small, and we can approximate the expectation of the *tanh* with the value of the *tanh* function at the expectation of the argument. Thus, we make the assumption that the expectation of a nonlinear function is the value of that function at the expectation of its argument. The resulting approximate kinetic equations will involve some terms of the form $\mathbf{E}(s_k q_l)$, for example.

If we suppose that all the spins s_p and q_p, $p \in \Lambda$, take values independently of the other spin values (statistical independence), then we can use the following approximation:

$$\mathbf{E}(s_k q_l) \cong \mathbf{E}(s_k)\mathbf{E}(q_l), \quad \text{for all } k,\, l. \tag{5.2.16}$$

Averaging out in (5.2.14) and (5.2.15), and using the above approximations, we finally obtain the system

$$\text{(ABV)} \begin{cases} \dfrac{du_k}{dt} = \dfrac{1}{2}\displaystyle\sum_{l\in N(k)} (u_l w_k + u_k w_l)\{u_l - u_k + \\ \qquad\qquad +(1 - u_l u_k)\tanh[\beta(Y_k - Y_l + 2J_{kl}(u_k - u_l))]\} \\ \dfrac{dw_k}{dt} = \dfrac{1}{2}\displaystyle\sum_{l\in N(k)} (w_l + w_k)\{w_l - w_k + \\ \qquad\qquad +(1 - w_l w_k)\tanh[\dfrac{\beta}{2}(Y_k - Y_l + J_{kl}(w_k - w_l))]\} \end{cases}$$

for all $k \in \Lambda$, where we have set:

$$u_i = \mathbf{E}(s_i), \quad w_i = \mathbf{E}(q_i)$$

and

$$Y_i = \mathbf{E}(\gamma_i) = \sum_{m\in N(i)} J_{im}(2u_m + w_m - 1), \qquad i = k, l. \tag{5.2.17}$$

Remark 5.1 This system is a generalization of the approximate kinetic equation (1.2.10) derived by O. Penrose in [86], representing the kinetic Ising model with Kawasaki (direct-exchange) dynamics. Note that in (1.2.10) the quantity u_k is the average of A-atoms at site k, and it is a value in the interval $[-1, 1]$. One can also derive this equation from the system formed by the exact equations (5.2.14) and (5.2.14) if we take $q_k = 1$, for all $k \in \Lambda$. Indeed, in this case we find that the system is equivalent to a single equation,

$$\frac{d}{dt}\mathbf{E}(s_k) = \frac{1}{2}\sum_{l\in N(k)} \mathbf{E}\{(s_l + s_k)[(s_l - s_k) + \\ +(1 - s_l s_k)\tanh(\beta(\gamma_k - \gamma_l + 2J_{kl}(s_k - s_l)))]\}, \tag{5.2.18}$$

where now

$$\gamma_p = \sum_{m \in N(p)} 2J_{pm}s_m, \quad \text{for all } p \in \Lambda.$$

But

$$(s_l + s_k)(s_l - s_k) = s_l - s_k$$

and

$$(s_l + s_k)(1 - s_l s_k) = (s_l - s_k)^2,$$

for all k, $l \in \Lambda$. The equation (5.2.18) can be written as

$$\frac{d}{dt}\mathbf{E}(s_k) = \frac{1}{2}\sum_{l \in N(k)} \{\mathbf{E}(s_l - s_k) + \mathbf{E}[(s_l - s_k)^2 \tanh(\beta(\gamma_k - \gamma_l + 2J_{kl}(s_k - s_l)))]\},$$

Changing the spin variable s to S, such that $S_k = 2s_k - 1 \in \{-1, 1\}$ for all lattice sites k, we get that

$$\gamma_p = \sum_{m \in N(p)} J_{pm}S_m := v_p, \quad \text{for all } p \in \Lambda.$$

and using the fact that

$$(S_l - S_k)^2 = 2(1 - S_l S_k), \quad \text{for all } k, l \in \Lambda,$$

we recover the equation (1.2.10).

Remark 5.2 It is not hard to show that the system (ABV) conserves mass, that is,

$$\frac{d}{dt}\sum_{k \in \Lambda} u_k = 0 \quad \text{and} \quad \frac{d}{dt}\sum_{k \in \Lambda} w_k = 0.$$

Indeed, if we denote by M_{lk} and, respectively, N_{lk} the following expressions

$$M_{lk} = \frac{1}{2}(u_l w_k + u_k w_l)\{u_l - u_k + (1 - u_l u_k)\tanh[\beta(Y_k - Y_l + 2J_{kl}(u_k - u_l))]\}$$

$$N_{lk} = \frac{1}{2}(w_l + w_k)\{w_l - w_k + (1 - w_l w_k)\tanh[\frac{\beta}{2}(Y_k - Y_l + J_{kl}(w_k - w_l))]\},$$

then it is obvious that

$$M_{lk} = -M_{kl} \text{ and } N_{lk} = -N_{kl}.$$

The system (ABV) becomes:

$$\begin{cases} \dfrac{du_k}{dt} = \displaystyle\sum_{l \in N(k)} M_{lk} \\ \dfrac{dw_k}{dt} = \displaystyle\sum_{l \in N(k)} N_{lk}, \quad k \in \Lambda. \end{cases}$$

Because $l \in N(k) \Longleftrightarrow k \in N(l)$, then we can write

$$\frac{d}{dt}\sum_{k\in\Lambda} u_k = \sum_{k\in\Lambda}\frac{du_k}{dt} = \sum_{k\in\Lambda}\sum_{l\in N(k)} M_{lk} = \sum_{l\in\Lambda}\sum_{k\in N(l)} M_{kl} = 0,$$

and

$$\frac{d}{dt}\sum_{k\in\Lambda} w_k = \sum_{k\in\Lambda}\frac{dw_k}{dt} = \sum_{k\in\Lambda}\sum_{l\in N(k)} N_{lk} = \sum_{l\in\Lambda}\sum_{k\in N(l)} N_{kl} = 0.$$

5.3 The Lyapunov function

Provided that all the interaction energies J_{kl} have the same value, which we denote by J, we show that for all $k \in \Lambda$ and $l \in N(k)$ the system (ABV) has a Lyapunov function, which can be interpreted as a free energy. Let us consider the function ϕ given by (1.2.13), whose derivative is

$$\phi'(z) = \operatorname{arctanh} z.$$

Consider now the following expression:

$$L(u,w) = -\frac{J}{4}\sum_{k\in\Lambda}\sum_{l\in N(k)}(2u_k + w_k)(2u_l + w_l) - \\ -J\sum_{k\in\Lambda}[u_k^2 + \frac{1}{4}w_k^2] + \frac{1}{\beta}\sum_{k\in\Lambda}[\phi(u_k) + \phi(w_k)]. \qquad (5.3.1)$$

We then have

$$\beta\frac{\partial L}{\partial u_k} = \phi'(u_k) - Z_k,$$

$$\beta\frac{\partial L}{\partial w_k} = \phi'(w_k) - \Theta_k,$$

for all $k \in \Lambda$, where by Z_k and Θ_k we have denoted the quantities

$$\begin{aligned} Z_k &= \beta J \sum_{m \in N(k)} (2u_m + w_m) + 2\beta J u_k \\ &= \beta(Y_k + 2Ju_k) + z\beta J, \end{aligned}$$

and

$$\begin{aligned} \Theta_k &= \frac{\beta}{2} J \sum_{m \in N(k)} (2u_m + w_m) + \frac{\beta}{2} J w_k \\ &= \frac{\beta}{2}(Y_k + Jw_k) + \frac{\beta}{2} zJ. \end{aligned}$$

Due to the relation $l \in N(k) \Longleftrightarrow k \in N(l)$ we have

$$\begin{aligned} \frac{dL}{dt} &= \sum_{k \in \Lambda} \frac{\partial L}{\partial u_k} \frac{du_k}{dt} + \sum_{k \in \Lambda} \frac{\partial L}{\partial w_k} \frac{dw_k}{dt} \\ &= \sum_{k \in \Lambda} \frac{\partial L}{\partial u_k} \sum_{l \in N(k)} M_{lk} + \sum_{k \in \Lambda} \frac{\partial L}{\partial w_k} \sum_{l \in N(k)} N_{lk} \\ &= \frac{1}{2} \sum_{k \in \Lambda} \sum_{l \in N(k)} [\frac{\partial L}{\partial u_k} - \frac{\partial L}{\partial u_l}] M_{lk} + \frac{1}{2} \sum_{k \in \Lambda} \sum_{l \in N(k)} [\frac{\partial L}{\partial w_k} - \frac{\partial L}{\partial w_l}] N_{lk}. \quad (5.3.2) \end{aligned}$$

We can rewrite M_{lk} in the following way:

$$\begin{aligned} M_{lk} &= \frac{1}{2}(u_l w_k + u_k w_l)(1 - u_l u_k)\{\frac{u_l - u_k}{1 - u_l u_k} + \tanh[\beta(Y_k - Y_l + 2J(u_k - u_l))]\} \\ &= \frac{1}{2}(u_l w_k + u_k w_l)(1 - u_l u_k)\{\tanh[\phi'(u_l) - \phi'(u_k)] + \tanh[Z_k - Z_l]\}. \end{aligned}$$

In a similar manner, N_{lk} is written as

$$\begin{aligned} N_{lk} &= \frac{1}{2}(w_l + w_k)(1 - w_l w_k)\{\frac{w_l - w_k}{1 - w_l w_k} + \tanh[\frac{\beta}{2}(Y_k - Y_l + J(w_k - w_l))]\} \\ &= \frac{1}{2}(w_l + w_k)(1 - w_l w_k)\{\tanh[\phi'(w_l) - \phi'(w_k)] + \tanh[\Theta_k - \Theta_l]\}. \end{aligned}$$

We now substitute the expressions of M_{lk} and N_{lk} into (5.3.2). Taking into account that $(u_l w_k + u_k w_l)$, $(w_l + w_k)$ and $(1 - u_l u_k)$, $(1 - w_l w_k)$ are all non-negative quantities, and $\alpha + \beta$ and $\tanh\alpha + \tanh\beta$ have the same sign for all α

and β, we obtain

$$\begin{aligned}\beta\frac{dL}{dt} = &-\frac{1}{4}\sum_{k\in\Lambda}\sum_{l\in N(k)}(u_l w_k + u_k w_l)(1-u_l u_k)[(\phi'(u_l)-\phi'(u_k))+(Z_k - Z_l)]\times \\ &\times\{\tanh[\phi'(u_l)-\phi'(u_k)]+\tanh[Z_k - Z_l]\} \\ &-\frac{1}{4}\sum_{k\in\Lambda}\sum_{l\in N(k)}(w_l + w_k)(1-w_l w_k)[(\phi'(w_l)-\phi'(w_k))+(\Theta_k - \Theta_l)]\times \\ &\times\{\tanh[\phi'(w_l)-\phi'(w_k)]+\tanh[\Theta_k - \Theta_l]\} \\ \leq\ &0. \end{aligned} \tag{5.3.3}$$

The equality in (5.3.3) takes place when

$$\begin{cases}\phi'(u_l)-\phi'(u_k)+Z_k - Z_l = 0 \\ \phi'(w_l)-\phi'(w_k)+\Theta_k - \Theta_l = 0,\end{cases} \tag{5.3.4}$$

for all $k \in \Lambda$ and $l \in N(k)$, which means that the pair of vectors (u, w) is the stationary solution of (ABV). Obviously, the function $L(u, w)$ is bounded from below, and thus L is a Lyapunov function for the system.

5.4 Critical temperature

In this section we show the existence of a critical value for β (which corresponds to a critical temperature) for each of the functionals $E_{Kaw}(u)$ and $L(u, w)$. We begin with $E_{Kaw}(u)$ given by (1.2.14), and we consider only the case of solutions for which all components are equal. In this case $E_{Kaw}(u)$ becomes

$$E(u) = N(\frac{1}{\beta}\phi(u) - \frac{z+1}{2}Ju^2).$$

We show the existence of β_c such that, below this critical point $E_{Kaw}(u)$ is convex, and the uniform state $u \equiv 0$ is the only minimizer. If $\beta > \beta_c$ then the global minimizer is a state $u = (u_1, u_2, \ldots, u_n)$ in which the components u_k can take two distinct values, -1 and 1.

Since

$$\frac{\partial E(u)}{\partial u} = N(\frac{1}{\beta}\phi'(u) - (z+1)Ju),$$

a critical value of $E(u)$ satisfies the equation

$$u = \tanh(\beta(z+1)Ju). \tag{5.4.1}$$

One can find a value β_c such that for $\beta < \beta_c$ we can approximate

$$\tanh(\beta(z+1)Ju) \cong \beta(z+1)Ju,$$

and (5.4.1) has only the trivial solution $u \equiv 0$. If $\beta > \beta_c$, then the equation (5.4.1) has three solutions,

$$u = 0, \quad u = -\theta, \quad u = \theta \qquad (\theta \in (0, 1]).$$

The points $u = -\theta$ and $u = \theta$ are the global minimizers of $E(u)$. Moreover, $\theta \to 1$ as $\beta \to \infty$ (see Figure 5.1).

In the case $u_k \equiv u$ and $w_k \equiv w$ for all $k \in \Lambda$, the functional $L(u, w)$ becomes:

$$\mathcal{L}(u, w) = -N[\frac{zJ}{4}(2u+w)^2 - Ju^2 - \frac{J}{4}w^2 + \frac{1}{\beta}(\phi(u) + \phi(w))]. \tag{5.4.2}$$

It turns out that there is a value β_c such that $\mathcal{L}(u, w)$ is convex for $\beta < \beta_c$, and $(u, w) \equiv (0, 0)$ is the only minimizer. For $\beta > \beta_c$ then the absolute minimum of $\mathcal{L}$ is realized for some values u^*, $w^* \in (0, 1]$ (see Figure 5.2).

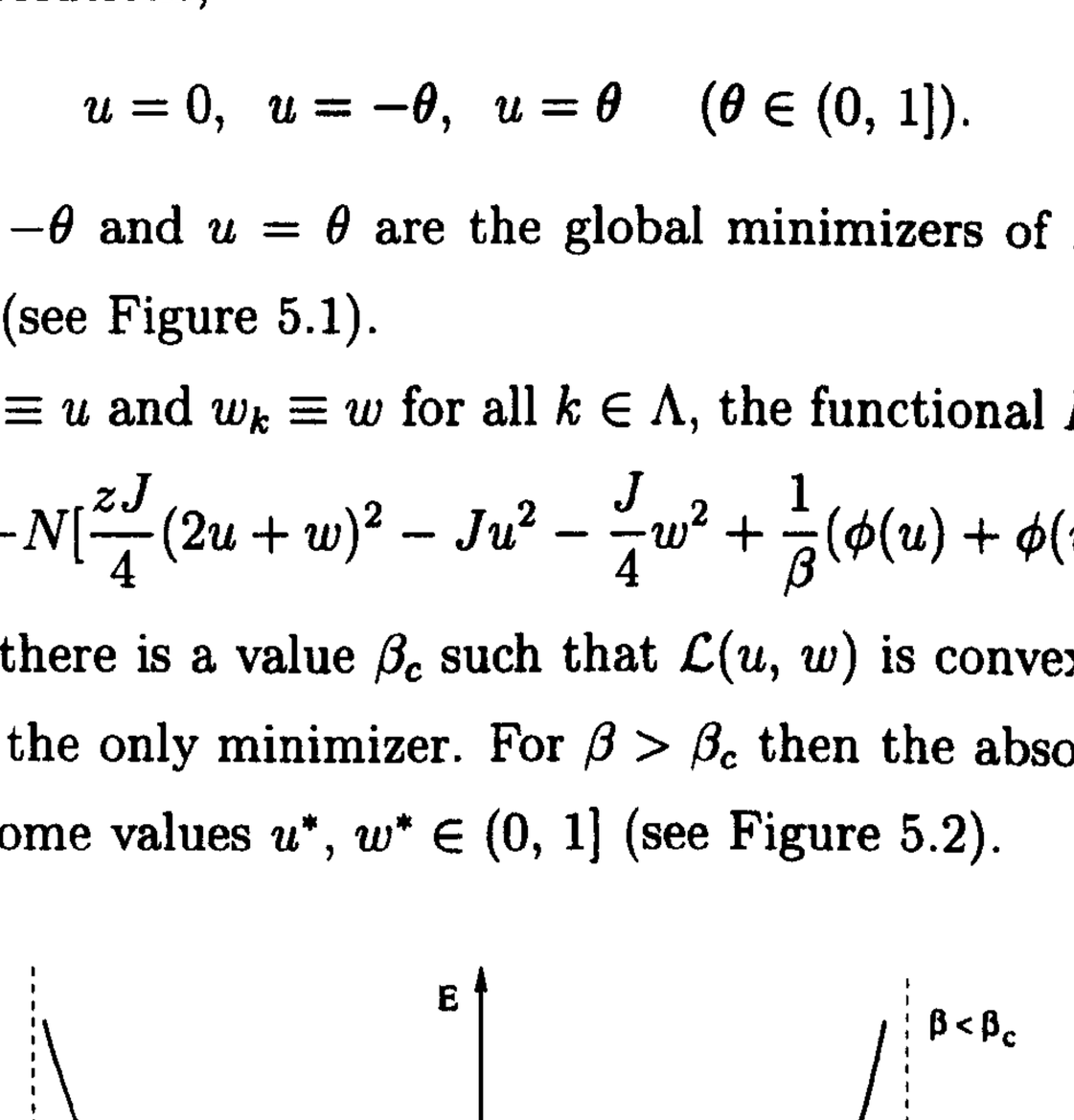

Figure 5.1: The function $E(u)$ for three different values of β.

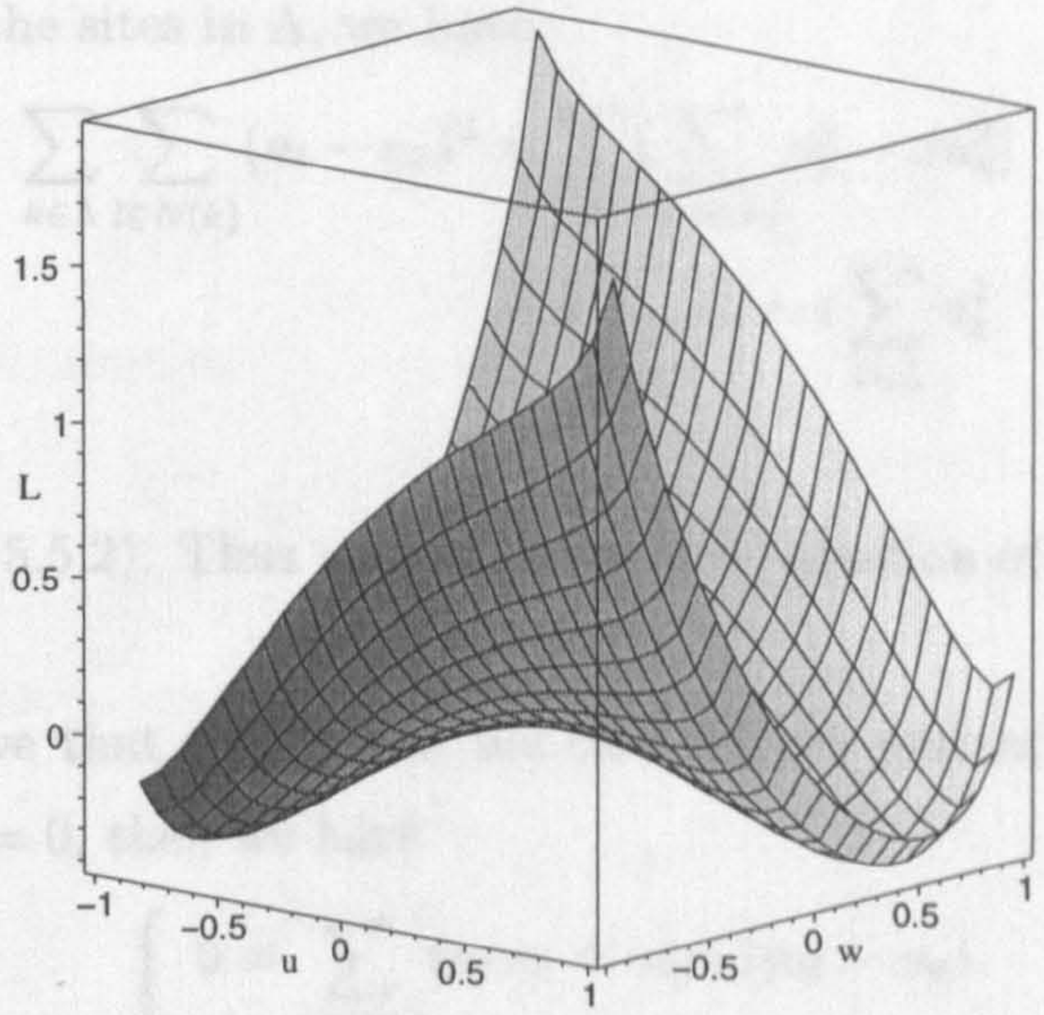

Figure 5.2: The function $\mathcal{L}(u, w)$ for $\beta > \beta_c$.

5.5 Infinite temperature

In the case of infinite temperature, which means $\beta = 0$, it is easy to prove that the problem of stationary solutions for (1.2.10), that is the following system

$$zu_k = \sum_{l \in N(k)} u_l, \quad k \in \Lambda, \tag{5.5.1}$$

has only the constant mass solution. Here z is the coordination number, i.e. the number of nearest neighbours of a lattice site. To show this, let us recall that in the Penrose model the variables u_k take values between -1 and 1. Since the variables $(u_k + 1)/2$ also satisfy (5.5.1), we may suppose $u_k \in [0, 1]$, for all k. Let us suppose that the system also admits a nonconstant solution. For this solution we have

$$\sum_{l \in N(k)} (u_l - u_k)^2 > 0, \quad \text{for all } k \in \Lambda. \tag{5.5.2}$$

On the other hand,

$$\begin{aligned} \sum_{l \in N(k)} (u_l - u_k)^2 &= z u_k^2 - 2u_k \sum_{l \in N(k)} u_l + \sum_{l \in N(k)} u_l^2 \\ &= -z u_k^2 + \sum_{l \in N(k)} u_l^2. \end{aligned}$$

Summing over all the sites in Λ, we have

$$\begin{aligned}\sum_{k\in\Lambda}\sum_{l\in N(k)}(u_l-u_k)^2 &= \sum_{k\in\Lambda}[\sum_{l\in N(k)}u_l^2 - zu_k^2]\\ &= z\sum_{k\in\Lambda}u_k^2 - z\sum_{k\in\Lambda}u_k^2\\ &= 0,\end{aligned}$$

which contradicts (5.5.2). Thus $u\equiv M_u$ is the only solution of (1.2.10) at infinite temperature.

We aim to prove that this is also the case for the system (ABV) at infinite temperature. If $\beta = 0$, then we have

$$(S)\begin{cases} 0 = \displaystyle\sum_{l\in N(k)}(u_lw_k + u_kw_l)(u_l-u_k)\\ 0 = \displaystyle\sum_{l\in N(k)}(w_l+w_k)(w_l-w_k),\end{cases}$$

for all $k\in\Lambda$, with the mass constraints

$$\sum_{k\in\Lambda}u_k = NM_u \text{ and } \sum_{k\in\Lambda}w_k = NM_w.$$

Here N denotes the number of sites of Λ and $0\le M_u, M_w\le 1$. We shall prove that if M_u and M_w $(M_w\neq 0)$ are given, then the system (S) has only the constant solution $(u,w)\equiv(M_u,M_w)$. Indeed, for an arbitrarily fixed site k, the last equation of (S) can be written as

$$\sum_{l\in N(k)}w_k^2 = \sum_{l\in N(k)}w_l^2$$

or, equivalently,

$$zw_k^2 = \sum_{l\in N(k)}w_l^2. \tag{5.5.3}$$

Obviously w_k cannot be 0 since this implies $w\equiv 0$, and thus $M_w = 0$. Using (5.5.3) we can write

$$\begin{aligned}\sum_{l\in N(k)}(w_l-w_k)^2 &= \sum_{l\in N(k)}w_l^2 - 2w_k\sum_{l\in N(k)}w_l + \sum_{l\in N(k)}w_k^2\\ &= 2zw_k^2 - 2w_k\sum_{l\in N(k)}w_l\\ &= 2w_k\sum_{l\in N(k)}(w_k-w_l).\end{aligned} \tag{5.5.4}$$

If we suppose that w is not constant, then

$$\sum_{l \in N(k)} (w_l - w_k)^2 > 0, \text{ for all } k \in \Lambda.$$

Since $w_k \neq 0$, (5.5.4) implies

$$\sum_{l \in N(k)} (w_k - w_l) > 0, \text{ for all } k \in \Lambda. \tag{5.5.5}$$

Taking in (5.5.5) the summation over all the sites k in Λ, we get

$$\sum_{k \in \Lambda} \sum_{l \in N(k)} (w_k - w_l) > 0,$$

which is false, since the mass constraint gives

$$\sum_{k \in \Lambda} \sum_{l \in N(k)} (w_k - w_l) = 0.$$

Thus, we can only have that w is constant for all the sites of the lattice. The first equation of (S) becomes now

$$\sum_{l \in N(k)} u_k^2 = \sum_{l \in N(k)} u_l^2,$$

and proceeding as we did for w, we get $u \equiv M_u$, and thus the system has only the constant solution.

5.6 Systems of discrete Cahn-Hilliard equations

Phase separation of alloys with two or more than two components was studied, among others, by Eyre in [40] using systems of Cahn-Hilliard equations. Let us consider a stable homogeneous alloy having $p+1$ $(p > 1)$ components, at high temperature. It has been experimentally observed that, when the temperature is lowered below a point where the homogeneous state is unstable, the components of the alloy show a tendency to separate into regions that have different compositions. Due to the mass conservation, the generalization of the Cahn-Hilliard

equation (2.2.19) gives a system of p coupled partial differential equations. If we take the order parameter to be

$$X = (X_1, X_2, \ldots, X_p), \quad \text{with } \sum_{i=1}^{p} X_1 = 1,$$

then the system of equations on a bounded domain $\Omega \subset \mathbb{R}$ can be written as

$$\frac{d}{dt}X(x) = \Delta[-\Gamma\Delta X(x) + \nabla_X F(X(x))], \qquad x \in \Omega,\ t > 0, \tag{5.6.1}$$

where

Γ is a symmetric $p \times p$ constant matrix with real components, and

$F : \mathbb{R}^p \longrightarrow \mathbb{R}$ is the bulk free energy.

For a particular case of the mobility matrix Γ, we will show here that we can get a similar system to (ABV) starting from the system (5.6.1). We consider the case of a ternary alloy, with

$$p = 2,\ X = [u,\ w]^T,\ F(X) = F(u, w),$$

and we take

$$\Gamma = \begin{bmatrix} 2J & J \\ J & J/2 \end{bmatrix},$$

where J is a positive scalar. The system (5.6.1) can be written as

$$\text{(C-H)} \begin{cases} \dfrac{d}{dt}u &= \Delta[\nabla_u F(u, w) - J(2\Delta u + \Delta w)] \\ \\ \dfrac{d}{dt}w &= \Delta[\nabla_w F(u, w) - \dfrac{J}{2}(2\Delta u + \Delta w)]. \end{cases}$$

If instead of $\Delta\xi$ we write $\sum_{l\in N(k)}(\xi_l-\xi_k)$, then the system (SC-H) has the discrete analogue

$$(D)\begin{cases}\dfrac{d}{dt}u_k &= \displaystyle\sum_{l\in N(k)}\{F_u(u_l,w_l)-F_u(u_k,w_k)+\sum_{m\in N(k)}J(2u_m+w_m)- \\ &\qquad -\sum_{n\in N(l)}J(2u_n+w_n)+2zJ(u_l-u_k)+zJ(w_l-w_k)\} \\ \dfrac{d}{dt}w_k &= \displaystyle\sum_{l\in N(k)}\{F_w(u_l,w_l)-F_w(u_k,w_k)+\frac{1}{2}\sum_{m\in N(k)}J(2u_m+w_m)- \\ &\qquad -\frac{1}{2}\sum_{n\in N(l)}J(2u_n+w_n)+zJ(u_l-u_k)+\frac{1}{2}zJ(w_l-w_k)\},\end{cases}$$

for all $k\in\Lambda$. Here z is the coordination number of the lattice.

We can show that the system (D) becomes similar to the system (ABV) provided we choose a suitable bulk free energy $F(u,w)$. We choose J to be as in the previous section, i.e., to be the common value of all nearest neighbour interactions, and $F(u,w)$ to be

$$F(u,w)=\beta^{-1}\phi(u)+\beta^{-1}\phi(w)-\frac{z}{4}J(2u+w)^2-Ju^2-\frac{1}{4}Jw^2.$$

For all $k\in\Lambda$, we have

$$F_u(u_k,w_k)=\beta^{-1}\phi'(u_k)-2(z+1)Ju_k-zJw_k$$

and

$$F_w(u_k,w_k)=\beta^{-1}\phi'(w_k)-\frac{1}{2}(z+1)Jw_k-zJu_k.$$

Substituting these expressions into (D) we obtain the system

$$(*)\begin{cases}\dfrac{d}{dt}u_k &= \beta^{-1}\displaystyle\sum_{l\in N(k)}\{\phi'(u_l)-\phi'(u_k)+\beta[Y_k-Y_l+2J(u_k-u_l)]\} \\ \dfrac{d}{dt}w_k &= \beta^{-1}\displaystyle\sum_{l\in N(k)}\{\phi'(w_l)-\phi'(w_k)+\beta[Y_k-Y_l+J(w_k-w_l)]\},\end{cases}$$

for all $k \in \Lambda$, where Y_k and Y_l are the expressions (5.2.17), with $J_{mn} = J$ for all $m, n \in \Lambda$. One can check that the functional $L(u, w)$ is a Lyapunov function for the system $(*)$. Using the notations used in Section 5.3, we have

$$\begin{aligned}\beta\frac{dL}{dt} &= -\frac{1}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)}[(\phi'(u_l)-\phi'(u_k))+(Z_k-Z_l)]^2 \\ &\quad -\frac{1}{2}\sum_{k\in\Lambda}\sum_{l\in N(k)}[(\phi'(w_l)-\phi'(w_k))+(\Theta_k-\Theta_l)]^2 \\ &\leq 0. \end{aligned} \tag{5.6.2}$$

The equality in (5.6.2) takes place when (u, w) satisfies (5.3.4). Since the systems (ABV) and $(*)$ have the same Lyapunov function, they will also have the same equilibrium solutions.

If we insert the positive factor $\beta(u_l w_k + u_k w_l)(1 - u_l u_k)$ in the first equation of $(*)$, the positive factor $\beta(w_l + w_k)(1 - w_l w_k)$ in the second one, and then replace the terms $\phi'(u_l) - \phi'(u_k)$, $\phi'(w_l) - \phi'(w_k)$, $\beta[Y_k - Y_l + 2J(u_k - u_l)]$ and $\beta[Y_k - Y_l + J(w_k - w_l)]$ by their hyperbolic tangents, we get the system (ABV).

5.7 A Vineyard-type approach to vacancy mediated diffusion

Based on the Vineyard formalism described in Section 1.2.4, we shall derive in this section mean-field models for ordering in a binary mixture via the vacancy-driven mechanism.

We consider a binary alloy with two kinds of atoms, A and B, and a small number of vacancies on a lattice Λ. For simplicity we shall regard vacancies as being a species of atoms. As in Section 1.2.4, by $N(x)$ we denote the set of all nearest neighbour sites of the site x, and we refer to $x + \delta$ as being an element of $N(x)$. Define $P_{\alpha_1,\alpha_2}(x, x + \delta; t)$ to be the probability that at a given time t, the sites x and $x + \delta$ are simultaneously occupied by atoms of type α_1 and α_2, respectively ($\alpha_{1,2} = A$, B, or V). The structural state of the alloy at a given temperature can be completely described by the set of multiparticle distribution

functions $P_{\alpha_1,\alpha_2}(x, x+\delta;\, t)$. We use here the vacancy mechanism explained in Section 5.2.

Consider a pair consisting of an A-atom at site x and a vacant nearest neighbour site at $x+\delta$. Under the influences of some other atoms of the lattice, the A-atom may jump to the site $x+\delta$ and the site x will become empty. For simplicity, we suppose that only the atoms occupying the nearest neighbour sites around the pair $(x,\, x+\delta)$ may exert an influence on the jump of the atom. Let us denote by $\{y\}$ the set of those nearest neighbour sites, by $\{X\}$ the set of atoms or vacancies occupying the sites $\{y\}$, and by $R_{AV}(\{X\})$, the rate at which the jump is completed under these circumstances. Likewise, let us denote by $R_{VA}(\{X\})$ the jump rate of an A-atom situated at $x+\delta$ to the vacant site x and having the same environmental set $\{X\}$. If $P_{AV\{X\}}(x, x+\delta, \{y\};\, t)$ denotes the probability of finding simultaneously an A-atom at x, a vacancy at $x+\delta$ and the set of atoms $\{X\}$ on the neighbouring sites $\{y\}$, then we can write the law for the rate of change of $P_A(x;\, t)$:

$$\frac{d}{dt}P_A(x;\, t) = \sum_{\delta}\sum_{\{X\}} P_{VA\{X\}}(x, x+\delta, \{y\};\, t)R_{VA}(\{X\}) - \sum_{\delta}\sum_{\{X\}} P_{AV\{X\}}(x, x+\delta, \{y\};\, t)R_{AV}(\{X\}). \qquad (5.7.1)$$

Using similar considerations for the jump of an B-atom to a nearest neighbour site $x+\delta$, we can write the analogous law for the change in $P_B(x;\, t)$:

$$\frac{d}{dt}P_B(x;\, t) = \sum_{\delta}\sum_{\{X\}} P_{VB\{X\}}(x, x+\delta, \{y\};\, t)R_{VB}(\{X\}) - \sum_{\delta}\sum_{\{X\}} P_{BV\{X\}}(x, x+\delta, \{y\};\, t)R_{BV}(\{X\}). \qquad (5.7.2)$$

In order to simplify the sums in the right hand side of equations (5.7.1) and (5.7.2), we use the simplest way to approximate the joint probabilities $P_{AV\{X\}}$, $P_{BV\{X\}}$, $P_{VA\{X\}}$, and $P_{VB\{X\}}$ by assuming statistical independence among occupation probabilities. For example, we approximate

$$P_{AV\{X\}}(x, x+\delta, \{y\}) \cong P_A(x)P_V(x+\delta)P_{X_1}(y_1)\ldots P_{X_n}(y_n),$$

where each y_i is an individual site in the set $\{y\}$, and X_i is an atom (A or B) or a vacancy occupying y_i $(i = 1, \ldots, n)$.

It only remains now to specify the jump rates $R_{AV}(\{X\})$. In the system there exist bond energies only between nearest neighbours, of amounts J_{AA}, J_{AB}, and J_{BB} between $A-A$, $A-B$ and $B-B$ pairs, respectively. All these quantities are considered to be non-negative and $J_{AB} = J_{BA}$. We suppose that the number of vacancies in the system is very small, such that if one of the given sites x or $x+\delta$ is empty, then there are no vacancies around this pair of sites. We also suppose from the beginning that $J_{AA} = J_{BB}$ and let

$$\epsilon = \frac{J_{AA} - J_{AB}}{2}.$$

We can see that ϵ is positive for an ordering system. The energy of a system configuration is the sum of all bond energies. Since $A-B$, $B-A$, $A-A$ and $B-B$ interchanges are not permitted, we need to find the contributions of pairs such as $A-V$ and $B-V$ to the total energy. Let us consider an A-atom at site x and a vacant nearest neighbour site $x+\delta$. Suppose that the site x has a number $n_A(x)$ of nearest neighbouring sites occupied by A-atoms and $n_B(x)$ nearest neighbouring sites occupied by B-atoms. Also, let $n_A(x+\delta)$ and $n_B(x+\delta)$ be the number of sites around the site $x+\delta$. Since we assumed that there are no vacancies around this pair, we see that (1.2.17) is satisfied in this case also.

The pair $A-V$ situated at $(x,\, x+\delta)$ contributes to the total energy by the amount

$$n_A(x)J_{AA} + n_B(x)J_{AB}.$$

After the jump of the A-atom to the vacant site is completed, the contribution of the new pair to the total energy will be

$$n_A(x+\delta)J_{AA} + n_B(x+\delta)J_{AB}.$$

Therefore, the net change in the energy is

$$\omega(x) = 2\varepsilon(n_A(x+\delta) - n_A(x)),$$

which characterizes the influence of the atoms situated in the nearest neighbour sites around the pair. The energy for an A-atom at site x to jump to a site $x+\delta$ is thus

$$U_A + 2\varepsilon(n_A(x+\delta) - n_A(x)),$$

where U_A is the activation energy, and the energy of an A-atom situated at site $x+\delta$ to jump to the vacancy at x is

$$U_A - 2\varepsilon(n_A(x+\delta) - n_A(x)).$$

Based on the general theory of chemical kinetics, Vineyard concluded that the jump rate of the pair depends on $\omega(x)$ and has the form

$$R_{AV}(\{X\}) = \nu_A e^{-\beta(U_A + 2\varepsilon(n_A(x+\delta) - n_A(x)))},$$

where ν_A is the vibrational frequency of an A-type atom. It is easy to check that $R_{AV}(\{X\})$ satisfy the detailed balance condition, condition which is also satisfied by

$$R_{AV}(\{X\}) = e^{-\beta\omega(x)},$$

which may be obtained by rescaling time and setting $\nu_A \exp(-\beta U_A) = 1$. For symmetry reasons we take

$$R_{BV}(\{X\}) = R_{AV}(\{X\}) := e^{-\beta\omega(x)},$$

and

$$R_{VB}(\{X\}) = R_{VA}(\{X\}) := e^{\beta\omega(x)}.$$

These are the forms of the jump rates that we shall consider from now on.

5.8 The averaged equations

We aim to simplify the equations (5.7.1) and (5.7.2) by averaging over the configurations. Let us define

$$N_A(x,t) = \begin{cases} 1, & \text{if the site } x \text{ is occupied by an } A\text{-atom at time } t \\ 0, & \text{otherwise,} \end{cases}$$

and the corresponding occupancies for B-atoms and vacancies, $N_B(x,t)$ and $N_V(x,t)$, respectively. Obviously,

$$N_A(x,t) + N_B(x,t) + N_V(x,t) = 1, \text{ for all } x \text{ and } t, \tag{5.8.1}$$

$$\langle N_A(x,t)\rangle = P_A(x,t), \quad \langle N_B(x,t)\rangle = P_B(x,t), \quad \langle N_V(x,t)\rangle = P_V(x,t),$$

where $\langle \cdot \rangle$ denotes the average (expected) value. By dropping the dependence on t, we can write the following equations:

$$\frac{d}{dt}\langle N_A(x)\rangle = \sum_\delta \langle N_V(x)N_A(x+\delta)e^{\beta\omega(x)} - N_V(x+\delta)N_A(x)e^{-\beta\omega(x)}\rangle \tag{5.8.2}$$

$$\frac{d}{dt}\langle N_B(x)\rangle = \sum_\delta \langle N_V(x)N_B(x+\delta)e^{\beta\omega(x)} - N_V(x+\delta)N_B(x)e^{-\beta\omega(x)}\rangle \tag{5.8.3}$$

We can rewrite (5.8.2) in the form

$$\frac{d}{dt}\langle N_A(x)\rangle = \sum_\delta \langle [N_V(x)N_A(x+\delta) + N_V(x+\delta)N_A(x)]\, p(x)e^{\beta\omega(x)p(x)}\rangle, \tag{5.8.4}$$

where

$$p(x) = N_A(x+\delta) - N_A(x).$$

Since $p \in \{-1, 0, 1\}$, the following identity holds:

$$pe^{pX} = p\cosh X(1 + p\tanh X). \tag{5.8.5}$$

Using this in (5.8.4) we obtain

$$\begin{aligned}
\frac{d}{dt}\langle N_A(x)\rangle &= \\
&= \sum_\delta \langle [N_V(x)N_A(x+\delta) + N_V(x+\delta)N_A(x)]\cosh(\beta\omega(x)) \times \\
&\qquad \times \{N_A(x+\delta) - N_A(x) + (N_A(x+\delta) - N_A(x))^2 \tanh(\beta\omega(x))\}\rangle \\
&= \sum_\delta \langle \cosh(\beta\omega(x))\,[N_V(x)N_A(x+\delta) + N_V(x+\delta)N_A(x)] \times \\
&\qquad \times \{N_A(x+\delta) - N_A(x) + (1 - N_A(x)N_A(x+\delta))\tanh(\beta\omega(x))\}\rangle,
\end{aligned} \tag{5.8.6}$$

where in (5.8.6) we have used the following identity valid for all x and $x+\delta$:

$$\begin{aligned}
&[N_V(x)N_A(x+\delta) + N_V(x+\delta)N_A(x)][N_A(x+\delta) - N_A(x)]^2 = \\
&= [N_V(x)N_A(x+\delta) + N_V(x+\delta)N_A(x)][1 - N_A(x)N_A(x+\delta)].
\end{aligned}$$

By adding (5.8.2) and (5.8.3) and using (5.8.1) we get

$$\frac{d}{dt}\langle N_V(x)\rangle =$$
$$= \sum_\delta \langle N_V(x+\delta)[N_A(x)+N_B(x)]e^{-\beta\omega} - N_V(x)[N_A(x+\delta)+N_B(x+\delta)]e^{\beta\omega}\rangle$$
$$= \sum_\delta \langle N_V(x+\delta)[1-N_V(x)]e^{-\beta\omega} - N_V(x)[1-N_V(x+\delta)]e^{\beta\omega}\rangle$$
$$= \sum_\delta \langle N_V(x+\delta)e^{-\beta\omega} - N_V(x)e^{\beta\omega}\rangle \qquad (\text{since } N_V(x)N_V(x+\delta)=0)$$
$$= \sum_\delta \langle q(x)e^{-\beta\omega(x)q(x)}\rangle, \qquad (5.8.7)$$

where

$$q(x) = N_V(x+\delta) - N_V(x) \in \{-1, 0, 1\}.$$

The identity (5.8.5) with q instead of p transforms (5.8.7) into

$$\frac{d}{dt}\langle N_V(x)\rangle =$$
$$= \sum_\delta \langle \cosh(\beta\omega)[N_V(x+\delta)-N_V(x)]\{1+[N_V(x+\delta)-N_V(x)]\tanh(\beta\omega)\}\rangle$$
$$= \sum_\delta \langle \cosh(\beta\omega)[N_V(x+\delta)+N_V(x)]\{N_V(x+\delta)-N_V(x)+$$
$$+[1-N_V(x)N_V(x+\delta)]\tanh(\beta\omega)\}\rangle. \qquad (5.8.8)$$

Let us use the following notation:

$$u(x,t) = P_A(x,t) = \langle N_A(x)\rangle, \quad x\in\Lambda, \quad \text{for all } t,$$

$$w(x,t) = P_V(x,t) = \langle N_V(x)\rangle, \quad x\in\Lambda, \quad \text{for all } t.$$

and

$$Y(x) = \sum_{\xi\neq\delta}[2u(x+\xi)+w(x+\xi)-1],$$
$$Y(x+\delta) = \sum_{\delta+\gamma\neq 0}[2u(x+\delta+\gamma)+w(x+\delta+\gamma)-1].$$

With this notation we have

$$\begin{aligned}\langle \omega(x) \rangle &= \varepsilon \langle n_A(x+\delta) - n_A(x) \rangle - \varepsilon \langle n_B(x+\delta) - n_B(x) \rangle \\ &= \varepsilon [\sum_{\delta+\gamma\neq 0} P_A(x+\delta+\gamma) - \sum_{\xi\neq\delta} P_A(x+\xi)] - \\ &\qquad -\varepsilon [\sum_{\delta+\gamma\neq 0} P_B(x+\delta+\gamma) - \sum_{\xi\neq\delta} P_B(x+\xi)] \\ &= \varepsilon [Y(x+\delta) - Y(x)].\end{aligned}$$

Averaging out in (5.8.6) and (5.8.8), and approximating the expectation of a nonlinear function by that function at the expectation of the argument, we finally get the following system

$$\text{(V)} \begin{cases} u_t(x) = \sum_{\delta} \cosh[\beta(Y(x+\delta) - Y(x))]\,[u(x)w(x+\delta) + w(x)u(x+\delta)] \times \\ \qquad \times\{\, u(x+\delta) - u(x) + [1 - u(x)u(x+\delta)] \tanh[\beta(Y(x+\delta) - Y(x))]\,\} \\ w_t(x) = \sum_{\delta} \cosh[\beta(Y(x+\delta) - Y(x))]\,[w(x) + w(x+\delta)]\{\, w(x+\delta) - w(x) + \\ \qquad +[1 - w(x)w(x+\delta)] \tanh[\beta(Y(x+\delta) - Y(x))]\,\} \end{cases}$$

where we have scaled the inverse temperature by $\beta \mapsto \varepsilon\beta$.

Remark 5.3 One can observe that this system is similar to (ABV), the difference being the hyperbolic cosine terms in both equations. The function $L(u, w)$ given by (5.3.1) is also the Lyapunov function for this the system.

Using the Vineyard formalism, M. Grinfeld and O. Penrose [60] have derived the averaged equations for both Glauber dynamics and Kawasaki dynamics. For Glauber dynamics the equation is

$$u_t = \cosh(\beta v)[-u + \tanh \beta v], \quad t > 0, \tag{5.8.9}$$

where

$$u(x, t) = 2P_A(x, t) - 1, \quad \text{and} \quad v(x, t) = \sum_{\delta} u(x+\delta, t),$$

which is similar to the equation (1.2.9), the difference being the mobility term $\cosh(\beta v)$. Also, in the case of direct exchange dynamics they found a similar equation to (1.2.10), the differences being again an hyperbolic cosine term.

An interesting question regarding these new models is whether the flows generated by the last system and (ABV), or by the equations (1.2.9) and (5.8.9) are topologically conjugate or not.

5.9 Numerical analysis

In this section we shall present the results of numerical simulations of the mean-field equations (1.2.10) and (ABV) using the explicit Euler scheme in one and two dimensions. In all computations we take $J_{kl} = 1$, for all k, l.

The one dimensional Euler scheme for the Kawasaki equation (1.2.10) is given by:

$$\begin{cases} \partial u_k^n = \frac{1}{2}\{u_{k-1}^n - u_k^n + (1 - u_{k-1}^n u_k^n)\tanh[\beta(u_{k+1}^n - u_{k-2}^n)] + \\ \qquad + u_{k+1}^n - u_k^n + (1 - u_{k+1}^n u_k^n)\tanh[\beta(u_{k-1}^n - u_{k+2}^n)]\}, \quad n = 1, 2, \ldots, \\ u_k^0 = u_0, \quad k = 1, 2, \ldots, N, \end{cases}$$

where

$$\partial u^n = \frac{u^{n+1} - u^n}{\Delta t}, \quad n = 1, 2, \ldots,$$

and N is the number of lattice sites, Δt is the time step size. The mass conservation condition (1.2.11) can be written as

$$\frac{1}{N}\sum_{k=1}^{N} u_k = M_u.$$

Experiment 1. We take $\beta = 0.2$, $\Delta t = 0.5$ and use 100 lattice points. We take the initial data u_0 (and consequently v_0) such that each component is a randomly generated value between -1 and $+1$. The time evolution of the solution $u = (u_1, u_2, \ldots, u_{100})$ (plotted with blue colour) is shown in Figure 5.3. The function drawn with red represents $v = -u$. The solution u appears to converge to the constant mass solution M_u of (1.2.10). In Figure (5.4) the Lyapunov function (1.2.14) is represented as a function of time. After the initial drop in

$L_{Kaw}(u)$, the Lyapunov function remains fairly constant for very short periods, periods which become longer with time, and finally the function attains its minimum when u becomes constant M_u.

Experiment 2. In this experiment the parameter β is increased to $\beta = 1$, the time step is taken to be $\Delta t = 0.005$ and the grid size $N = 15$. We consider the same type of initial data as in *Experiment 1.* The evolutions of u (blue) and $v = -u$ (red) are represented in Figure 5.5. We observe that domains where $u = -1$ or $u = 1$ appear and the solution undergoes long periods of very slow evolution. This very slow motion is consistent with the results of J. Carr and R. L. Pego [21], where they discovered an exponentially slow evolution in the case of the Allen-Cahn equation (2.2.14). The smaller scale domains appear to shrink with time and finally the solution will coarsen to a phase separated state which is monotonic and minimizes the Lyapunov function (1.2.14) represented in Figure 5.6.

Experiment 3. We perform a two dimensional experiment for (1.2.10) on a 20×20 lattice. The initial data u_0 is taken to be a matrix with elements randomly generated values between -1 and 1. The time step is $\Delta t = 0.1 \times 10^{-4}$ and $\beta = 1$. We represent in Figure 5.7 the initial data u_0 and the evolution of the solution to (1.2.10) at four different times: 10^3, 10^4, 10^5 and 10^6. As in the previous experiment, we observe the appearance of phase domains where u takes the values ± 1, the coarsening process being again very slow.

The one-dimensional explicit Euler scheme for the equation for vacancy-mediated diffusion, (ABV), is

$$\begin{cases} \partial u^n = \frac{1}{2}\{(u^n_{k-1}w^n_k + w^n_{k-1}u^n_k)[u^n_{k-1} - u^n_k + (1 - u^n_{k-1}u^n_k)\tanh\beta(2u^n_{k+1} - 2u^n_{k-2} + \\ \qquad + w^n_{k+1} + w^n_{k-1} - w^n_k - w^n_{k-2})] + (u^n_{k+1}w^n_k + w^n_{k+1}u^n_k)[u^n_{k+1} - u^n_k + \\ \qquad + (1 - u^n_{k+1}u^n_k)\tanh\beta(2u^n_{k-1} - 2u^n_{k+2} + w^n_{k-1} + w^n_{k+1} - w^n_k - w^n_{k+2})]\} \\ \partial w^n = \frac{1}{2}\{(w^n_{k-1} + w^n_k)[w^n_{k-1} - w^n_k + (1 - w^n_{k-1}w^n_k)\tanh\frac{\beta}{2}(2u^n_{k-1} + 2u^n_{k+1} - \\ \qquad - 2u^n_{k-2} - 2u^n_k + w^n_{k+1} - w^n_{k-2})] + (w^n_{k+1} + w^n_k)[w^n_{k+1} - w^n_k + \\ \qquad + (1 - w^n_{k+1}w^n_k)\tanh\frac{\beta}{2}(2u^n_{k-1} + 2u^n_{k+1} - 2u^n_{k-2} - 2u^n_k + w^n_{k-1} - w^n_{k+2})]\} \end{cases}$$

for $k = 1, 2, \ldots, N$ and $n = 1, 2, \ldots,$ with

$$\begin{cases} u^0_k = u_0, \\ w^0_k = w_0, \quad k = 1, 2, \ldots, N. \end{cases}$$

Experiment 4. We take $\beta = 0.1$, $\Delta t = 0.01$ and the grid size $N = 15$. The initial data (u_0, v_0, w_0) is such that the components of u_0 are randomly generated values within the interval $[0, 0.8]$, w_0 has components which are random numbers between 0 and 0.15, and thus the components of $v_0 = 1 - u_0 - w_0$ are values between 0.05 and 1. The evolution of the solution of (ABV) having this initial data is represented in Figure 5.9 (we use blue to represent the average of A-atoms, red for the average of B-atoms and green for vacancies). One can observe the appearance of regions with A-rich and B-rich phases, with a higher average of vacancies in the interfaces that separate these regions. Finally, in this case the solution decays to the constant solution $u = (M_u, M_v, M_w)$. In Figure 5.10 we have plotted the Lyapunov function $L(u, w)$ given by (5.3.1) as a function of time. We see that this function decreases in time along the solutions of (ABV).

Experiment 5. The parameter β is increased to $\beta = 0.51$, $\Delta t = 5 \times 10^{-4}$ and we take $N = 12$ lattice points. The initial data (u_0, v_0, w_0) is as in the previous experiment. One can observe again the appearance of regions with A-rich and B-rich phases which coarsen in time. The system evolves very slowly towards a minimum of the Lyapunov functional drawn in Figure 5.12.

Based on these experiments we conjecture that there is a critical value for β, say β_c (which corresponds to a critical temperature T_c) such that if $0 \leq \beta < \beta_c$ the solution of the equation (1.2.10) or of the system (ABV) decays to the constant mass solution which is stable, and if $\beta > \beta_c$, then the solution evolves towards phase separation into domains having either A-atoms or B-atoms.

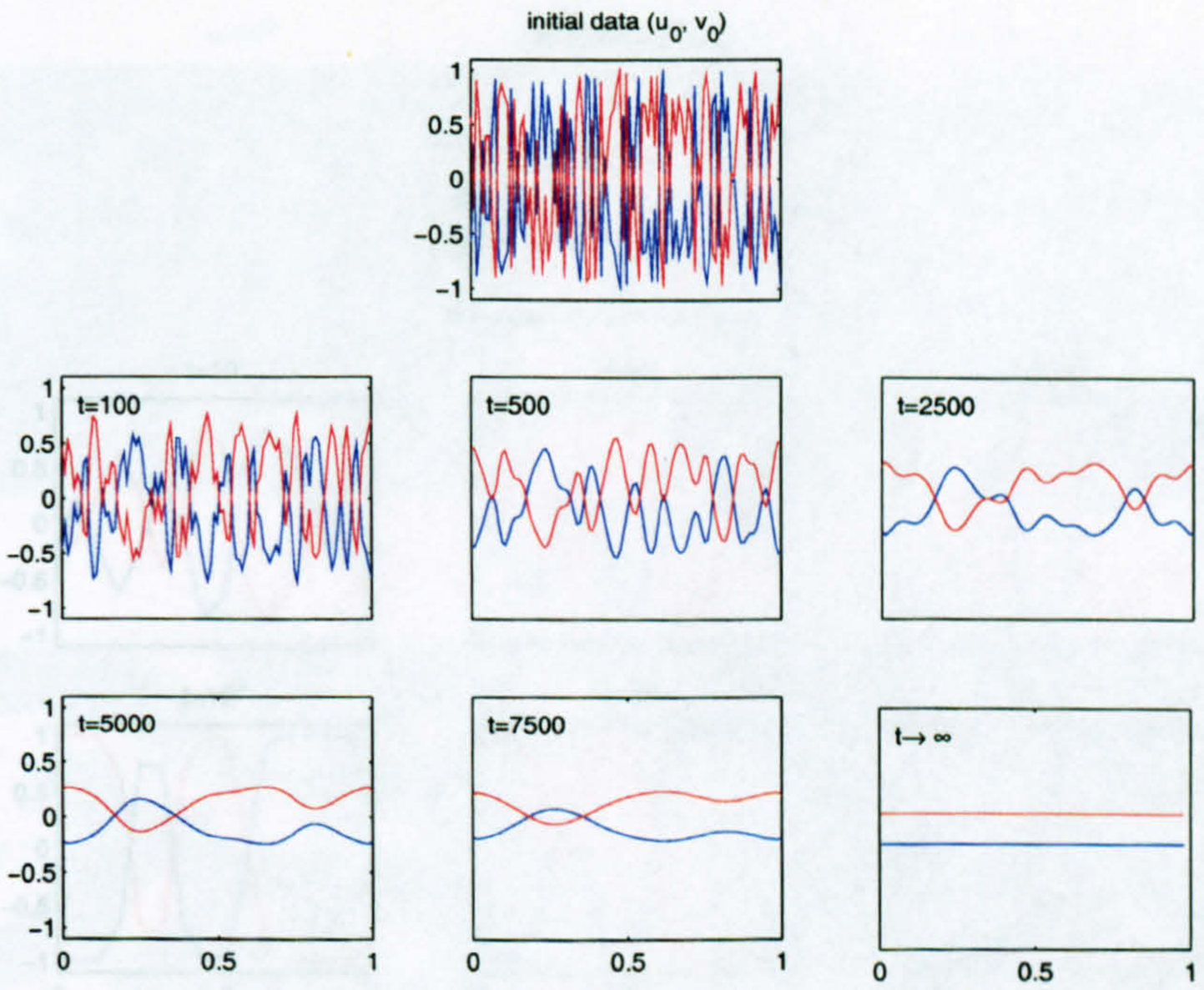

Figure 5.3: The solution of (1.2.10) with $\beta = 0.2$ at different values of time t (the grid size $N = 100$).

Figure 5.4: The Lyapunov functional (1.2.14) against time ($\beta = 0.2$, $N = 100$).

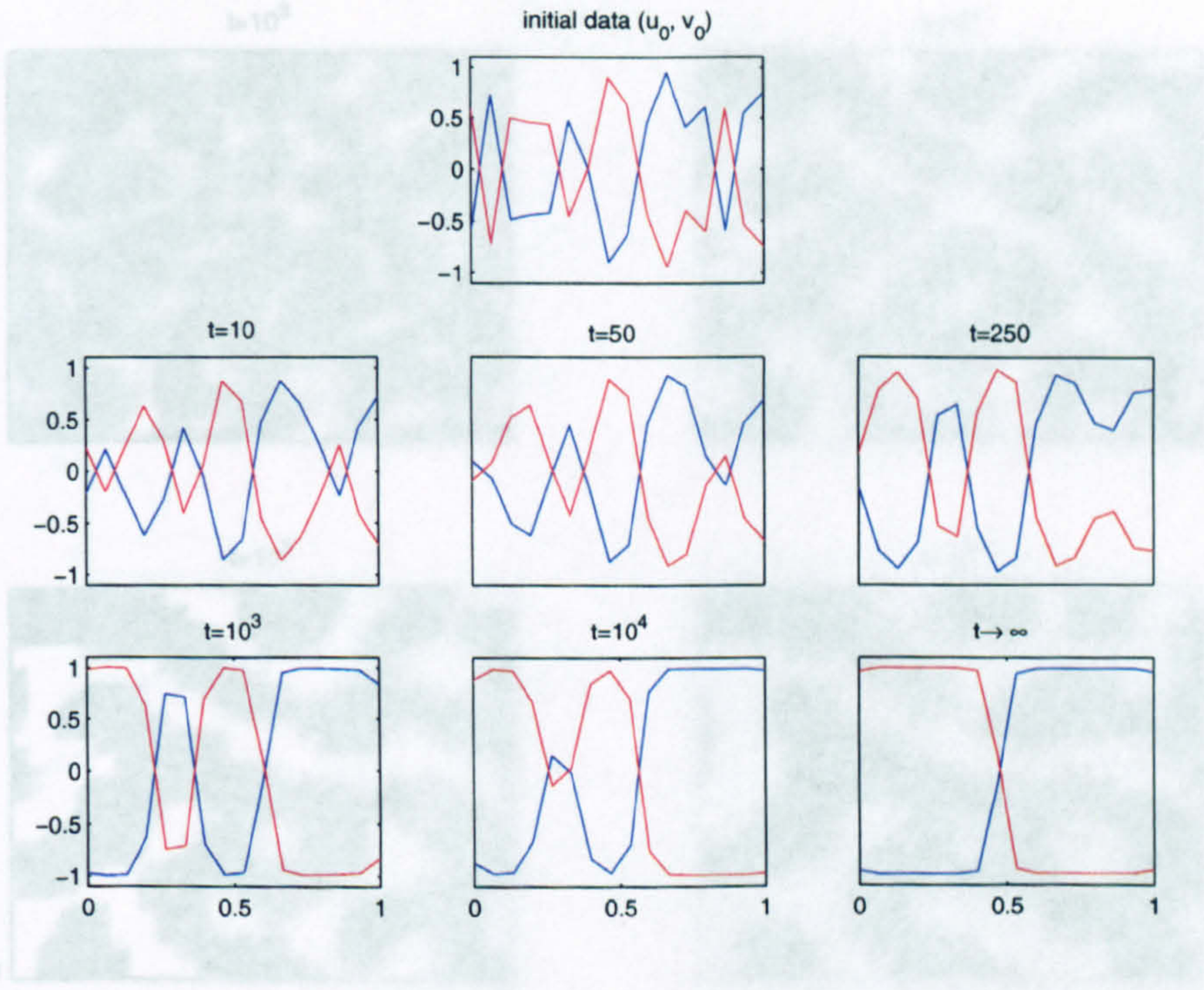

Figure 5.5: The solution of (1.2.10) with $\beta = 1$ at different values of time t (the grid size $N = 15$).

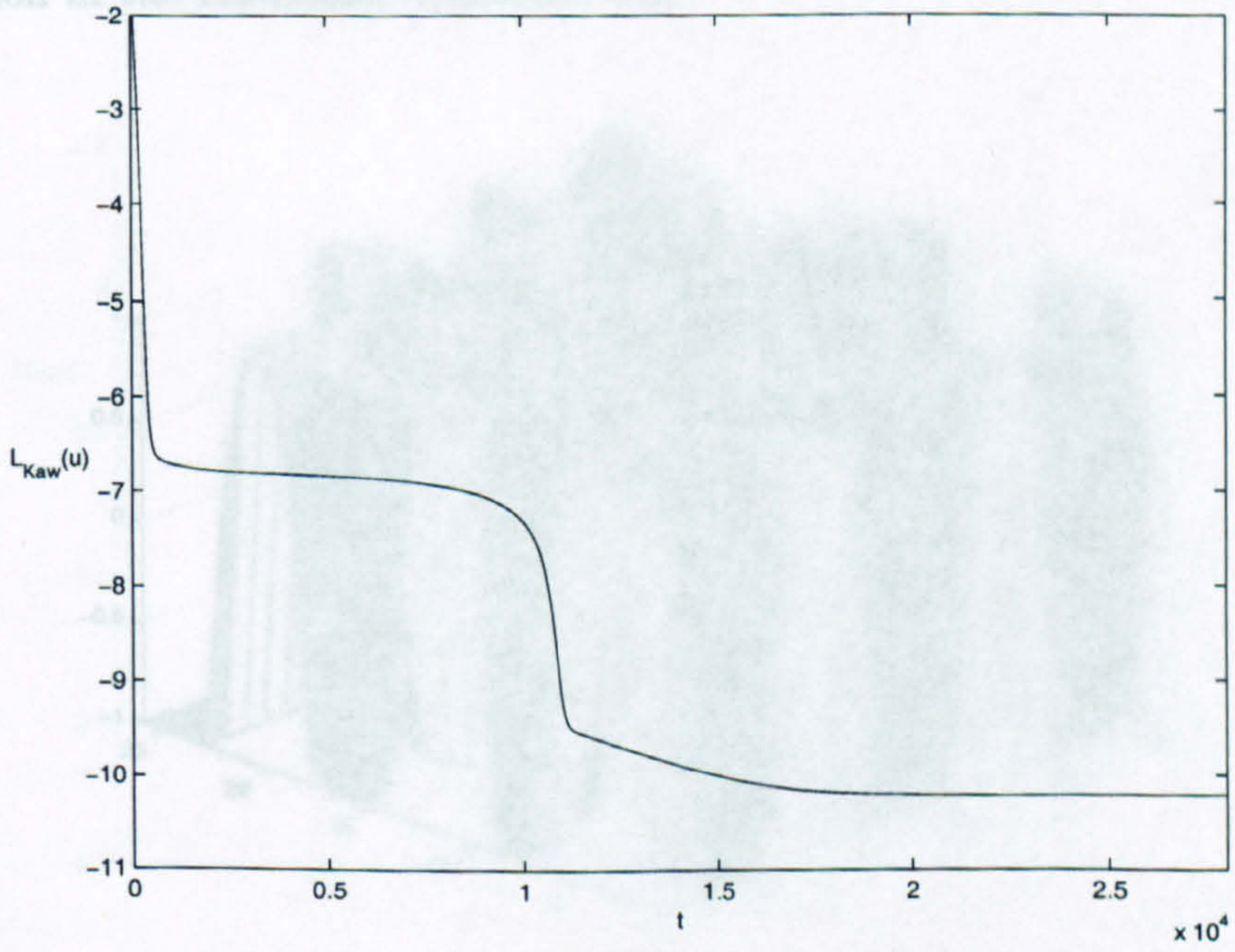

Figure 5.6: The Lyapunov functional (1.2.14) against time ($\beta = 1$, $N = 15$).

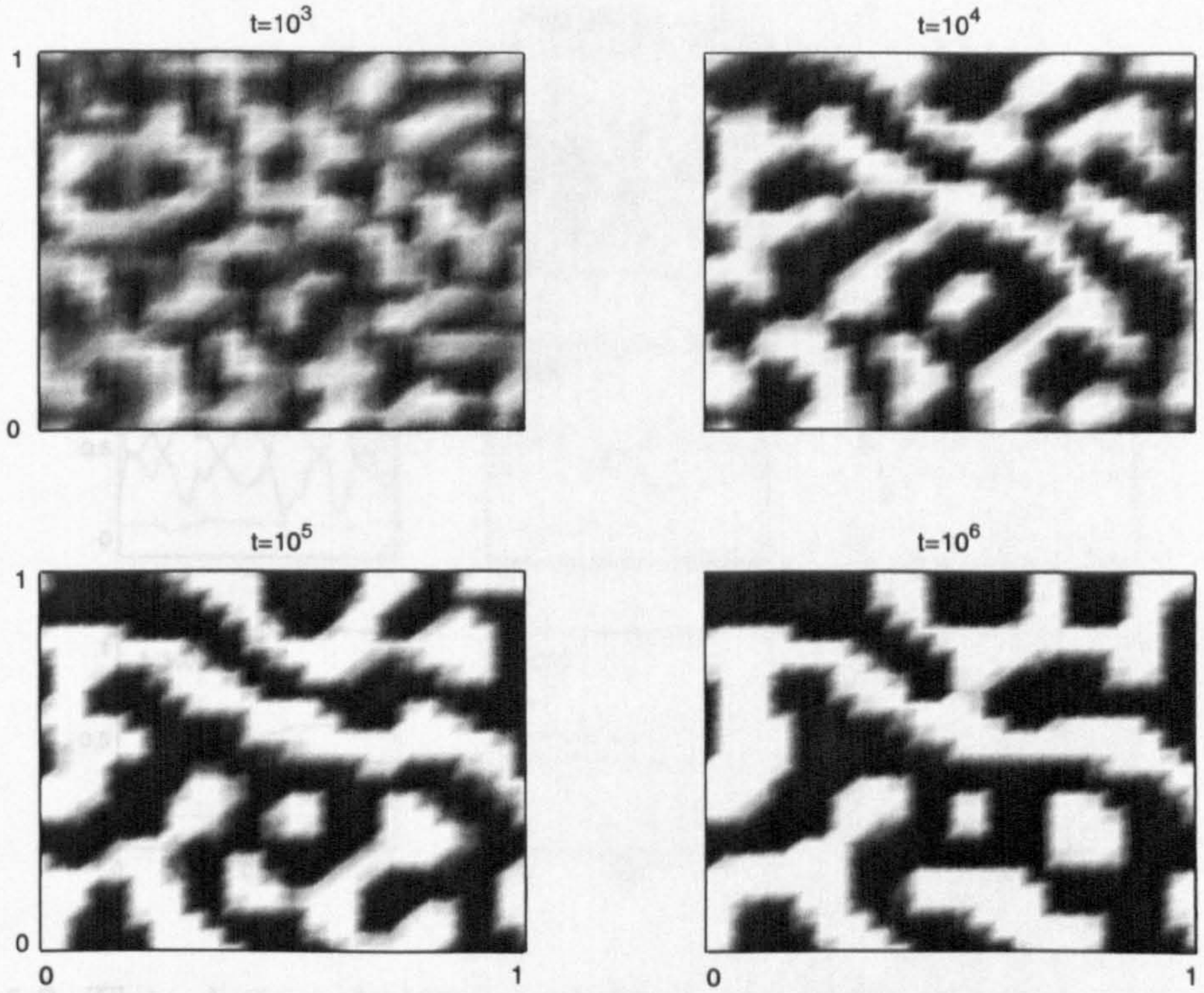

Figure 5.7: Morphological pattern formation and evolution during spinodal decomposition in the Kawasaki dynamics case.

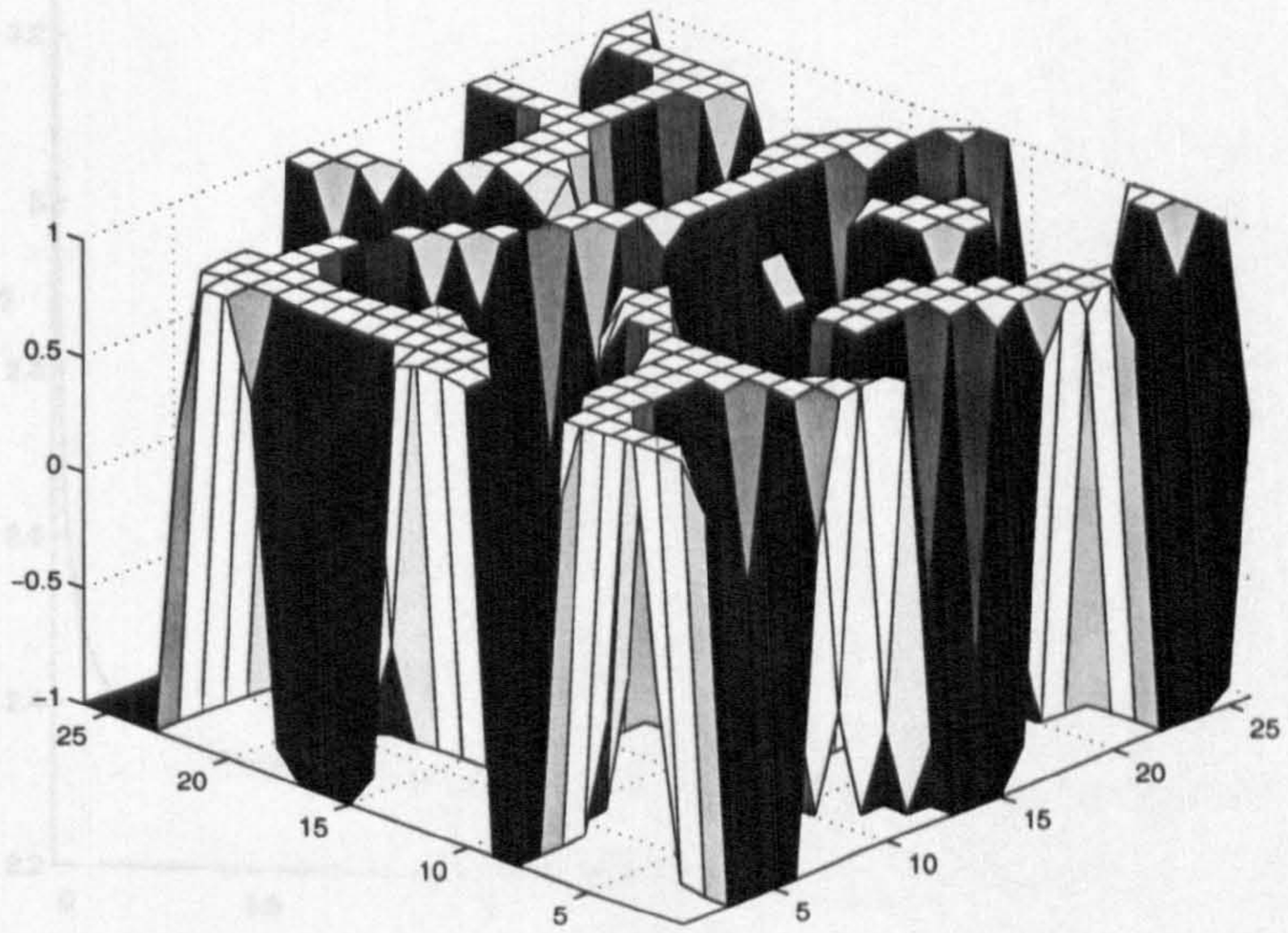

Figure 5.8: The solution of (ABV) at time $t = 10^6$ ($\beta = 1$).

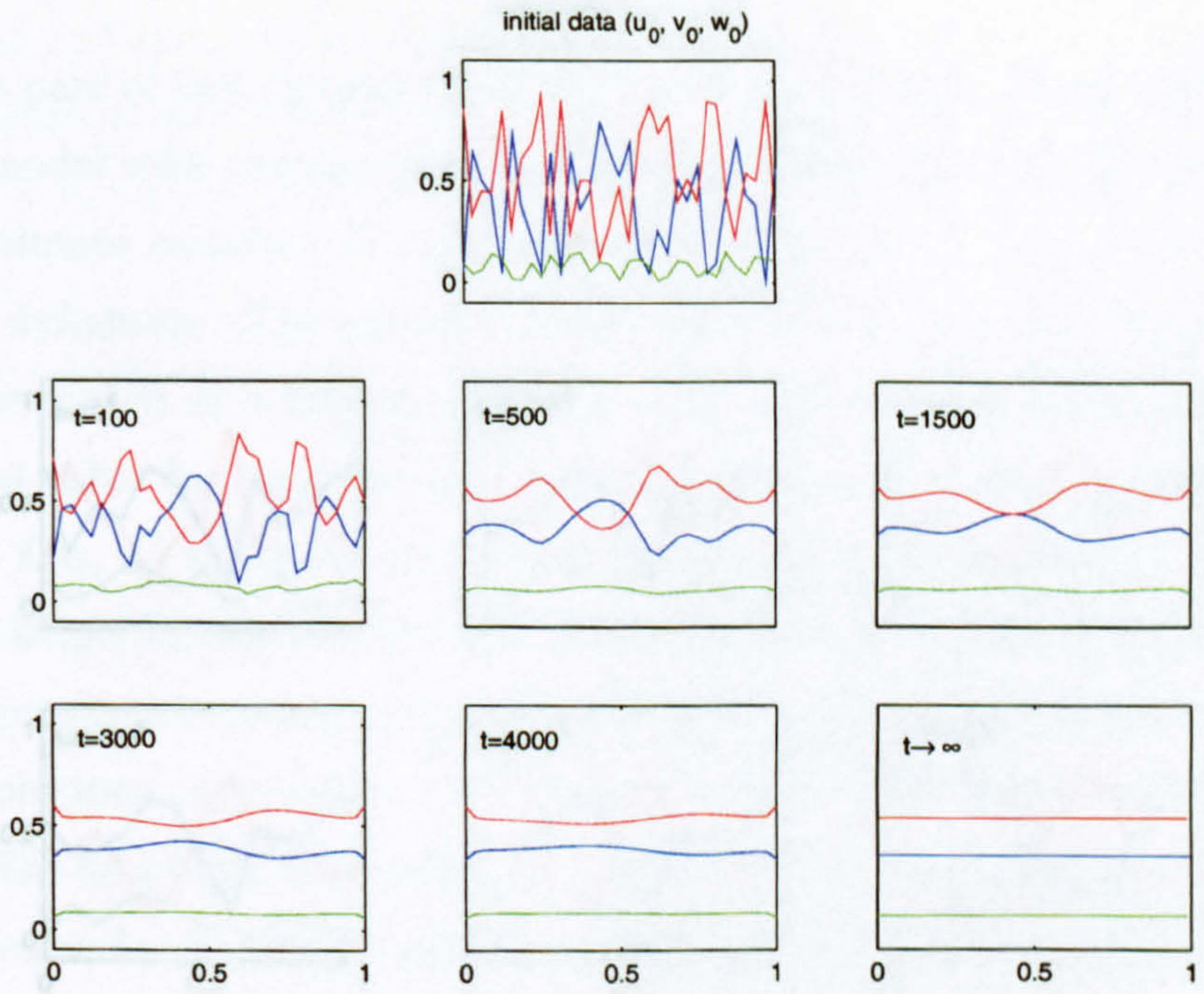

Figure 5.9: The solution of (ABV) with $\beta = 0.1$ at different values of time t (the grid size $N = 32$).

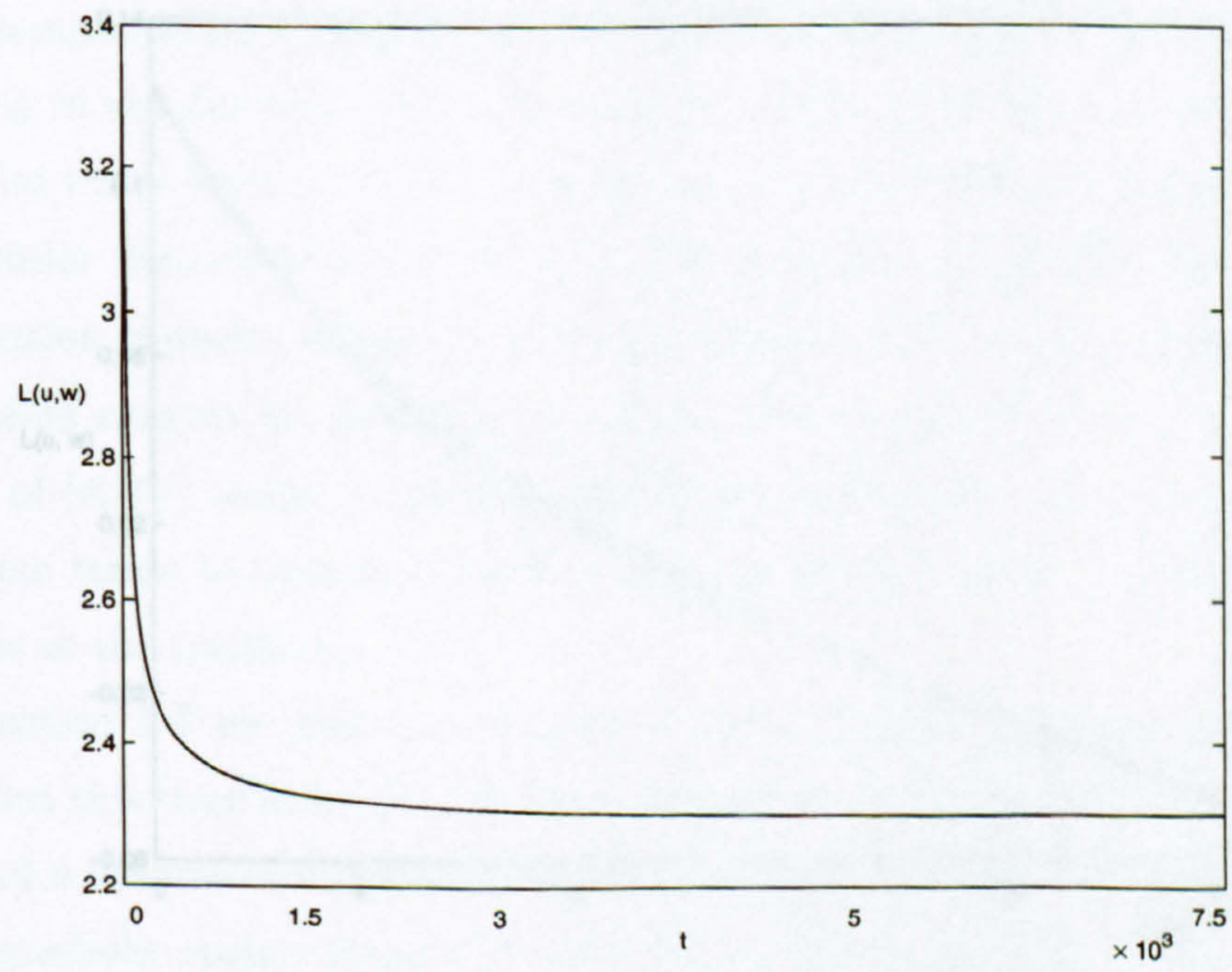

Figure 5.10: The Lyapunov functional (5.3.1) against time ($\beta = 0.1$, $N = 32$).

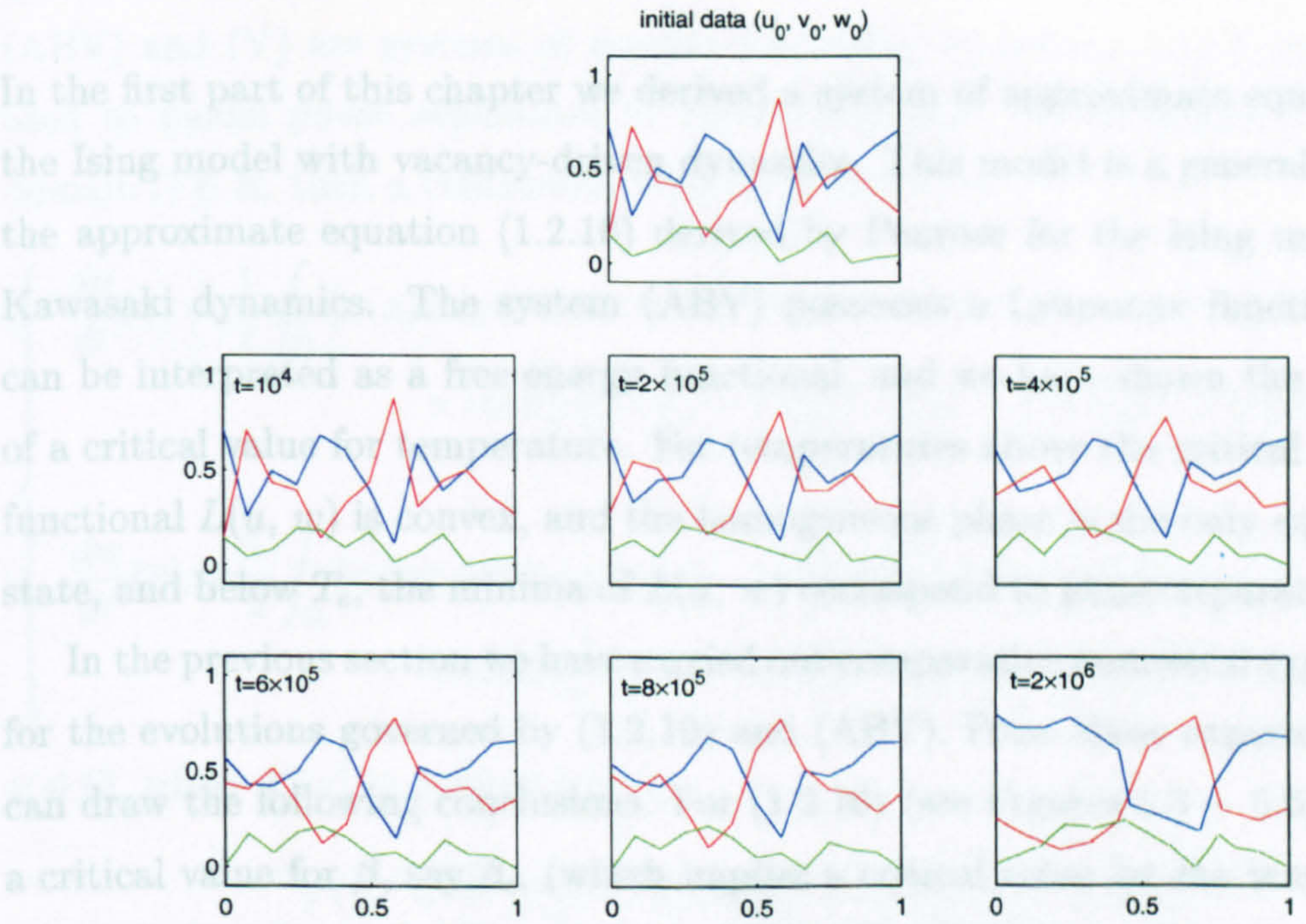

Figure 5.11: The solution of (ABV) with $\beta = 0.51$ at different values of time t (the grid size $N = 12$).

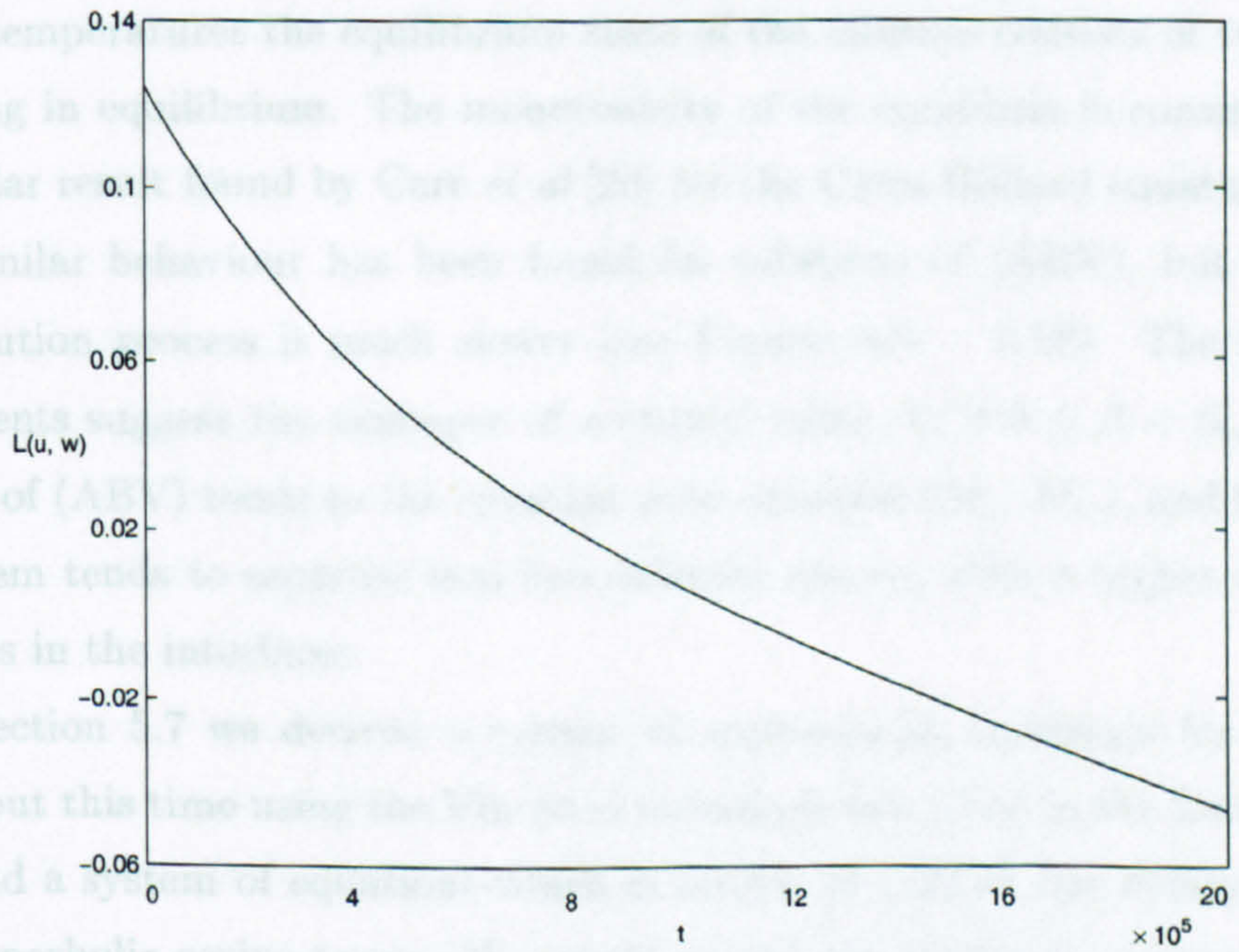

Figure 5.12: The Lyapunov functional (5.3.1) against time ($\beta = 0.51$, $N = 12$).

5.10 Conclusions

In the first part of this chapter we derived a system of approximate equations for the Ising model with vacancy-driven dynamics. This model is a generalization of the approximate equation (1.2.10) derived by Penrose for the Ising model with Kawasaki dynamics. The system (ABV) possesses a Lyapunov function which can be interpreted as a free energy functional, and we have shown the existence of a critical value for temperature. For temperatures above the critical point the functional $L(u, w)$ is convex, and the homogeneous phase is the only equilibrium state, and below T_c, the minima of $L(u, w)$ correspond to phase separated states.

In the previous section we have carried out comparative numerical experiments for the evolutions governed by (1.2.10) and (ABV). From these experiments one can draw the following conclusions. For (1.2.10) (see Figures 5.3 – 5.6), there is a critical value for β, say β_c, (which implies a critical value for the temperature, T_c) such that if $0 \leq \beta < \beta_c$ solutions of (1.2.10) will decay to the constant mass solution, which is the global minimizer of the Lyapunov function (1.2.14). For $\beta > \beta_c$, solutions converge to a monotonic steady state solution. This means that at high temperatures the system will tend to the homogeneous state, and for low enough temperatures the equilibrium state of the mixture consists of two phases coexisting in equilibrium. The monotonicity of the equilibria is consistent with the similar result found by Carr *et al* [20] for the Cahn-Hilliard equation.

A similar behaviour has been found for solutions of (ABV), but this time the evolution process is much slower (see Figures 5.9 – 5.12). The numerical experiments suggest the existence of a critical value β_c; if $0 \leq \beta < \beta_c$, then the solution of (ABV) tends to the constant mass solution (M_u, M_w), and for $\beta > \beta_c$ the system tends to separate into two different phases, with a higher average of vacancies in the interfaces.

In Section 5.7 we derived a system of approximate equations for the same model, but this time using the Vineyard formalism described in the first Chapter. We found a system of equations which is similar to (ABV), the difference being some hyperbolic cosine terms. We would expect the evolution of this system to be similar to that of the system (ABV).

At the end of this chapter, let us mention that the continuous versions of (ABV) and (V) are systems of integro-differential equations, which can also be used to model phase separation in binary mixtures. If the lattice Λ covers a domain $\Omega \in \mathbb{R}$, then a continuous version of (ABV) is

$$\begin{cases} \dfrac{du}{dt}(x) = \dfrac{1}{2}\displaystyle\int_\Omega (u(x)w(y) + u(y)w(x))\{u(y) - u(x) + (1 - u(x)u(y))\times \\ \qquad\qquad \times \tanh[\beta(Y(x) - Y(y) - J(|x-y|)(w(x) - w(y)))]\}\, dy \\ \\ \dfrac{dw}{dt}(x) = \dfrac{1}{2}\displaystyle\int_\Omega (w(x) + w(y))\{w(y) - w(x) + (1 - w(x)w(y))\times \\ \qquad\qquad \times \tanh[\dfrac{\beta}{2}(Y(x) - Y(y) - 2J(|x-y|)(u(x) - u(y)))]\}\, dy, \end{cases}$$

$x \in \Omega$, where $Y(x)$ is defined here by

$$Y(x) = \int_\Omega J(|x-z|)(2u(z) + w(z))\, dz, \qquad x \in \Omega. \tag{5.10.1}$$

We easily see that this system conserves mass, since the expressions under the integral are anti-symmetric in x and y.

Chapter 6

Conclusions and further work

In Chapter 3 we were concerned with a nonlocal version of the Allen-Cahn equation. We proved that (3.3.1) generates a flow in $L^\infty(\Omega)$ and we have discussed some qualitative properties of the solutions to the nonlocal Allen-Cahn equation. We found that, unlike the solutions of the Allen-Cahn equation, solutions of (3.3.1) do not coarsen at all if the strength of interactions between particles in the system is small enough. We proved this result only for $J \geq 0$, and the main key in the proof was the comparison principle. It is not clear yet what happens with the coarsening process if the assumption $J \geq 0$ is removed, since the comparison principle is no longer valid in this case. Although the non-coarsening property of solutions was proved under the restrictive condition $\|u_0\| < 1$, the result of Theorem 3.22 remains valid if this restriction is removed, but we are unable to use the same technique in proving the result (basically, we cannot use the comparison principle). For $\|u_0\| > 1$, one can prove the non-coarsening of solutions to (3.3.1) using rather different ideas. For example, one can try to show that the number of zeros of solutions to (3.3.1) with small enough γ does not decrease to zero when $t \to \infty$. Alternatively, one can follow the ideas of Fife and Wang [48] in proving Theorem 3.21.

We did not prove a stabilisation result for (3.3.1). In the case of equation (2.2.14), which generates a gradient system on $L^2(\Omega)$, a stabilisation result follows from the general theory of such systems (e. g., see [24], [64]). This theory cannot

be applied to (3.3.1) because of the lack of compactness of the positive semi-orbits.

In Section (3.6) we approximated the flow generated by the nonlocal Allen-Cahn equation by flows obtained using Padé approximants. Everything about the equations $(\mathcal{P}_n)$ is open. It would be interesting to see whether the equilibrium solutions corresponding to (P_n), and those of (3.3.1) have the same structural properties (cardinality, stability).

Chapter 4 deals with nonlocal mass conserving versions of the following equations: the Rubinstein-Sternberg equation (2.2.20), the Cahn-Hilliard equation (2.2.19) and the viscous Cahn-Hilliard equation (2.2.15). These equations are derived as constrained gradient flows of the free energy functional (3.3.9). We consider their associated initial value problems, and prove existence and uniqueness results. As we have shown in the last part of Section 3.6, one can obtain the Cahn-Hilliard equation (2.2.19) from (4.3.1) by using Padé approximation.

All the nonlocal equations studied in Chapter 4 have the same stationary solutions, properties of which are discussed in Section 4.5. We find similarities between the properties of these solutions and the equilibria of (2.2.19), such as the unique constant mass solution for γ or $|M|$ large enough.

The numerical experiments show solutions to (4.2.1) and (4.3.1) do not coarsen if the parameters γ or ϵ are small enough, a phenomenon which is not common to the local equations. The maximum principle does not hold here, hence the arguments of Chapter 3 are not applicable.

We believe that these equations were never considered before; everything about their properties remains open. One also can consider systems of nonlocal Cahn-Hilliard equations, which can model phase separation in multi-component alloys, or systems of nonlocal Allen-Cahn and Cahn-Hilliard equations. One can also consider non-local Allen-Cahn or Cahn-Hilliard equations in which the mobility term (see Definition 2.12) is not constant.

In Chapter 5 we derived mean-field equations directly from a microscopic model on a lattice. The model approximately represents the average behaviour of the Ising model, where the atoms are allowed to exchange places in the lattice via a vacancy mechanism. The proposed system is discussed in parallel with the mean-field equation derived by Penrose which represents the kinetic Ising model

with direct exchange dynamics. As in the case of the Penrose equation (1.2.10), we found that (ABV) possesses a Lyapunov function, which can be interpreted as a free energy. The numerical experiments show the existence of a critical temperature for this functional; above this critical point the system decays to the constant mass solution, and for temperatures below T_c the mixture tends to separate into two phases.

In the last part of the chapter we use the Vineyard formalism for the vacancy-interchange model to derive a similar system of equations to (ABV). It would be interesting to see whether the the flow generated by the new system is topologically conjugate to the flow generated by (ABV).

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