

Coarsening Dynamics for the Cahn-Hilliard Equation

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Coarsening Dynamics for the Cahn-Hilliard Equation

Research Thesis

Submitted in partial fulfillment
of the requirements for the degree of Master of Science in
Applied Mathematics

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Submitted to the Senate of the Technion - Israel Institute of Technology
Tishrei 5770 Haifa October 2009

This research thesis was done under the supervision of Prof. Amy Novick-Cohen and Prof. Michael Zhittomirskii of the Department of Mathematics.

The financial support and encouragement of the Technion is greatly appreciated.

I am greatly indebted to Prof. Amy Novick-Cohen for her devoted guidance and for her cooperation and support at every stage of this work.

I thank Michael Assa, Vadim Derkach and Dr. Eliahu Levy for helping me with the technicalities of the computer typing.

This work is dedicated to my dear Family and to the memory of my Parents.

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Abstract

The Cahn-Hilliard (C-H) equation has been proposed as a model to describe the evolution of a conserved concentration field during the spontaneously phase separation of a binary fluid mixture below the critical temperature. After a mixture, in which both components are initially uniformly present in the domain under consideration, undergoes rapid cooling below the critical temperature, the homogenous state becomes unstable.

As a result, phase separation occurs and the domain splits into regions which are rich in one component and poor in the other. So, by decreasing the temperature, the system enters a non-equilibrium state, and rapidly decomposes into microstructural regions with different phases. Each phase is characterized by a distinct composition of the individual components, in a manner which reduces the bulk chemical energy of the system. This formation of micro-structure occurs on a very fast time scale, and is called spinodal decomposition. Later the dominant length scale of the micro-structure grows in a process known as a coarsening.

The purpose of this thesis is to understand coarsening phenomena which occur during phase separation rigorously and to investigate the power laws which govern the evolution of the dominant length scale. Our main goal is to find the most appropriate upper bounds for the coarsening rates and how these upper bounds depend on the parameters of the system, such as the temperature, and the mean concentration.

Chapter 1

Introduction

The Cahn-Hilliard equation for

$$u_t = \Delta(-\epsilon^2 \Delta u + f'(u)), \quad t > 0, \quad x \in \mathbb{R}^n, \quad (1 - 1 - 1)$$

was proposed for the first time in around 1958 [1, 2] as a model for the process of phase separation of a binary alloy below the critical temperature. It has since appeared in many other contexts ranging from micro-film dynamics, the dynamics of polymer flow, as well as in bio-film structure formation, population dynamics, river bed formation, and image processing. More recently it has appeared in nano-technology, in models for the stellar dynamics, as well as in the theory of galaxy formation as a model for the evolution of two components of inter-galactic material [12]. Hence, the Cahn-Hilliard equation appears not only in the context of modeling very small structures such as in the micro-structure of binary alloys and bio-films, but also in modeling some very large structures, such as certain patterning features which have been seen in the inner "B" ring which revolves around the planet Saturn [6]. Since this equation appears in a wide diversity of applications, many scientists, engineers, and mathematicians have had considerable interest in this equation, and much attention has been paid to this equation. These efforts have included analytical studies, see e.g. F.Otto & R. V. Kohn [3], asymptotic studies, see e.g. A.Novick-Cohen [22], and numerical studies, see e.g. V. Calupecy [7], H. Garcke, M. Rumpf & U. Weikkard [37]. In short, the Cahn-Hilliard equation constitutes one of the leading models for studying phase separation in isothermal, isotropic mixtures. The details of phase separation of course depend on the initial ratio of the components of the mixture.

If initially both components are present in basically the same ratio or in roughly similar proportions, a process called spinodal decomposition takes place, followed afterwards by coarsening [7], as we shall explain in the coming chapters. If initially the mixture contains significantly higher amount of one component, nuclei of the poorer component form and grow, and phase separation takes place via a process called nucleation and growth. Generally speaking, the physical and chemical properties of the compound from which the mixture is made determine the nature of the phase separation process.

The function $u(t, x)$ in [11],[23] represents the difference of the two concentrations in a two component system,

$$u = c_A - c_B.$$

Hence, u should satisfy $u \in [-1, 1]$, and the function $f : \mathbb{R} \rightarrow \mathbb{R}$ should be of "bistable type" with three simple zeros. Alternatively $u(t, x)$ can represent the concentration of one of the two components of the mixture, say $u = c_a$, and therefore should satisfy $u \in [0, 1]$. Assuming that $u(t, x)$ represents the concentration of one of the two components and that the total mass of each of the two components is constant, the Cahn-Hilliard equation may be written as

$$u_t = \nabla M(u) \nabla \mu, \quad \mu = f'(u) - \varepsilon^2 \Delta u, \quad (1-1-2)$$

where the coefficient $M(u) \geq 0$ denotes the mobility. Roughly speaking, there are two kinds of mobilities. The first one is constant mobility with, say $M(u) = 1$. Another kind, $M(u) = u(1 - u)$, is known as degenerate mobility, which we will try to analyze rigorously. In (1-1-2), μ is the chemical potential, $f(u)$ is the homogeneous free energy and the parameter ε is an interaction length. Equation (1-1-2) with $M(u) = u(1 - u)$ constitutes a degenerate parabolic equation, and it is referred to as the Cahn-Hilliard equation with degenerate mobility.

The predicted behavior has a characteristic length scale $\ell(t)$ which grows as t^α , with $\alpha = 1/4$ or $1/3$, although other values have also been proposed for the manner in which the length scale grows during the various stages of the coarsening process. Recent studies have shown the influence of anisotropy on the dynamics of coarsening. Computer simulations [24] show that if the in dimension $d = 2$ is modified to include arbitrary surface tension anisotropy, the asymptotic late stage-scaling growth law $\ell(t) \sim t^{1/3}$ remains unchanged. The structure factor $S(k, t)$ is bound into angular wedges and is found to exhibit distinct behavior in each wedge, indicating that the asymptotic domain structure is indeed anisotropic. A simple linear analysis about an unstable homogeneous equilibrium of the one dimensional Cahn-Hilliard equation gives heuristic evidence that most solutions that start with initial data near such a constant unstable equilibrium state exhibit spinodal decomposition [12].

The case of constant mobility is well investigated and a number of numerical schemes have been proposed based on both finite difference as well as finite element method [38]. The degenerate mobility case is more complicated. A nonlinear multi-grid method is a method that was proposed in order to solve the Cahn-Hilliard equation numerically. The power law

$$\ell(t) \sim t^{1/3} \quad (1-1-3)$$

has been demonstrated (rigorously), and is known as the Lifshitz-Slyozov law [6]. Moreover it has been verified by numerical simulations. Algebraic growth laws, such as

$$\ell(t) \sim t^{1/4},$$

can also be associated with surface diffusion dynamics [10]. The Cahn-Hilliard equation has the associated Lyapunov functional

$$F[u] = \int \left[\frac{1}{4}(u^2 - 1)^2 + \frac{\varepsilon^2}{2} |\nabla u|^2 \right]. \quad (1-1-4)$$

Extending the ideas of Kohn and Otto to obtain specific upper bounds for the limiting coarsening dynamics is one of the goals of this thesis.

Cahn, Elliott & Novick-Cohen [13] have considered the Cahn-Hilliard equation with mobility which vanishes in the pure phases $u = 0$ and $u = 1$, and which is based on the free energy functional

$$F = \int_{\Omega} f(u) + \frac{\varepsilon^2}{2} |\nabla u|^2 dx \quad (1-1-5)$$

with

$$f(u) = \theta g(u) - \frac{1}{2} \alpha u^2,$$

and

$$g(u) = u \ln u + (1 - u) \ln(1 - u) \quad (1-1-6)$$

where θ is temperature and $g(u)$ represents the entropy of the system. For

$$0 < \theta < \theta_{crit},$$

where $\theta_{crit} := \alpha$, $f(u)$ is a double well potential. By using the time scale $\tau = \varepsilon^2 t$, they showed that formal asymptotics indicate that the interface moves by minus the surface Laplacian of the mean curvature. The formal asymptotic analysis is appropriate for the description of the late time behavior during which the system is dominated by a finite number of regions in which locally energy minimizing phases prevail.

Chapter 2

Physical background

2.1 Phase separation

Phase separation can be understood in terms of phase diagrams based on classical thermodynamical considerations, as developed by Gibbs in 1873 [26]. If a system contains two components which are in equilibrium, then their chemical potentials are equal, i.e $\mu_1 = \mu_2$. The chemical potential, in other words, the partial molar Gibbs free energy, assumes a crucial role in determining the equation of state. The Gibbs free energy satisfies the thermodynamical relation $G = H - TS$, where H is the enthalpy, T denotes temperature, and S is the entropy. G can be expanded locally at or near equilibrium in term of the thermodynamic state variables. The Gibbs chemical potential is given by $\mu = \frac{\partial G}{\partial N}$. But in a closed system at constant temperature and pressure, it is appropriate to work with Helmholtz free energy rather than with the Gibbs free energy. A similar thermodynamic relation is $F = U - TS$, where F is the Helmholtz free energy and U denotes the internal energy. From these thermodynamic relations we can get that

$$dF = \left. \frac{\partial F}{\partial p} \right|_T dp + \left. \frac{\partial F}{\partial T} \right|_p dT + \sum \left. \frac{\partial F}{\partial N_i} \right|_p dN_i, \quad (2-1-1)$$

$$\mu_i = \left. \frac{\partial F}{\partial N_i} \right|_p. \quad (2-1-2)$$

Two decades after Gibbs' suggestions, Van der Waals in 1893 proposed the functional in (1-1-4), [19]. This has proved to be a good model for the free energy of binary systems (mixtures). Over sixty years later Cahn-Hilliard, [1, 2] independently derived this functional which contains a gradient term and a non-convex integral functional, and which has characteristic singular limits. Cahn and Hilliard derived from this functional the following equation

$$\frac{\partial u}{\partial t} = \Delta(-\varepsilon^2 \Delta u + f'(u)), \quad (x, t) \in \Omega, \quad (2-1-3)$$

where Ω is a bounded open subset of \mathbb{R}^n . This is an evolutionary equation induced by (1-1-4) through a generalization of Fick's law. Linear analysis of equation (2-1-3) suggests what we shall

call Spinodal Decomposition as we shall discuss in the next paragraph.

The quantity

$$\mu = f'(u) - \varepsilon^2 \Delta u$$

can be identified as the chemical potential, which we have mentioned above, and ε is the length of the transitional regions between domains during phase separation. Moreover, the Cahn-Hilliard equation may be written in the form

$$u_t = -\nabla \cdot J, \tag{2-1-4}$$

which is an equation of continuity which reflects the fact that matter is conserved, and J here denotes the mass flux (current) which is assumed to be orthogonal to the boundary, $J \cdot n = 0$. This differs from the Allen-Cahn equation for phase domain coarsening, which is an evolution equation for a non conserved order parameter. The mass flux (current) which is orthogonal to the boundary satisfies

$$J = -M(u) \nabla [f'(u) - \varepsilon^2 \nabla^2 u], \tag{2-1-5}$$

$M(u)$ is known as the internal diffusion coefficient or the mobility, and $M(u)$ is assumed to be non-negative, $M(u) \geq 0$, [13]. Moreover $f(u)$ is the homogenous contribution to the free energy, and $n \cdot \nabla u = 0$ on $\partial\Omega(x, t)$ where n is an exterior normal to $\partial\Omega$. From (2-1-4) and (2-1-5) we see the Cahn-Hilliard equation which describes the evolution of a conserved concentration during the phase separation,

$$\frac{\partial u}{\partial t} = \nabla \cdot M(u) \nabla [f'(u) - \varepsilon^2 \nabla^2 u]. \tag{2-1-6}$$

The Cahn-Hilliard equation can be derived from the free energy functional F ,

$$F[u] = \int_{\Omega} (f(u) + \varepsilon^2 |\nabla u|^2) dx. \tag{2-1-7}$$

The first term in (2-1-7) is the free energy of a homogenous solution, the second term is a gradient energy term, and F is taken to be defined on a bounded domain $\Omega \subset \mathbb{R}^n$, where $\partial\Omega \subset \mathbb{R}$ is assumed to have a sufficiently smooth boundary $\partial\Omega$, and with suitable boundary conditions prescribed on $\partial\Omega$.

If we assume that

$$f(u) = \frac{1}{4}(u^2 - 1)^2,$$

and $M(u) = 1$, then

$$u_t = \nabla^2 [(u^3 - u) - \varepsilon^2 \nabla^2 u]. \tag{2-1-8}$$

As we have indicated, phase separation generally occurs when a nearly uniform mixture of a binary alloy is quenched below a certain critical temperature where the uniform mixture becomes unstable. Immediately after the quench a micro-structure of two spatially separated phases with different concentrations develops. In the later stages of the evolution on a much longer time scale than the initial stages of separation, the structure becomes coarser, either by merging of particles or by the growth of bigger particles at the expense of smaller ones [38].

Phase separation has also been studied for multi-component systems. In particular, the linear stability of a system of Cahn-Hilliard equation with a concentration dependent mobility matrix has been studied. By using numerical simulations these equations could be used to see whether or not phase separation is predicted, as well as the nature of the phase separation. While the phase diagrams can vary in their levels of complexity, a simplest phase diagram can be prescribed which can already describe phase separation can be seen in Fig. 2.1, which is taken from A. Novick-Cohen's paper (1985). Above the coexistence curve the system is stable, below it phase separation may occur. At critical temperature and concentration, the system separates into the coexistence concentrations, c_1 and c_2 .

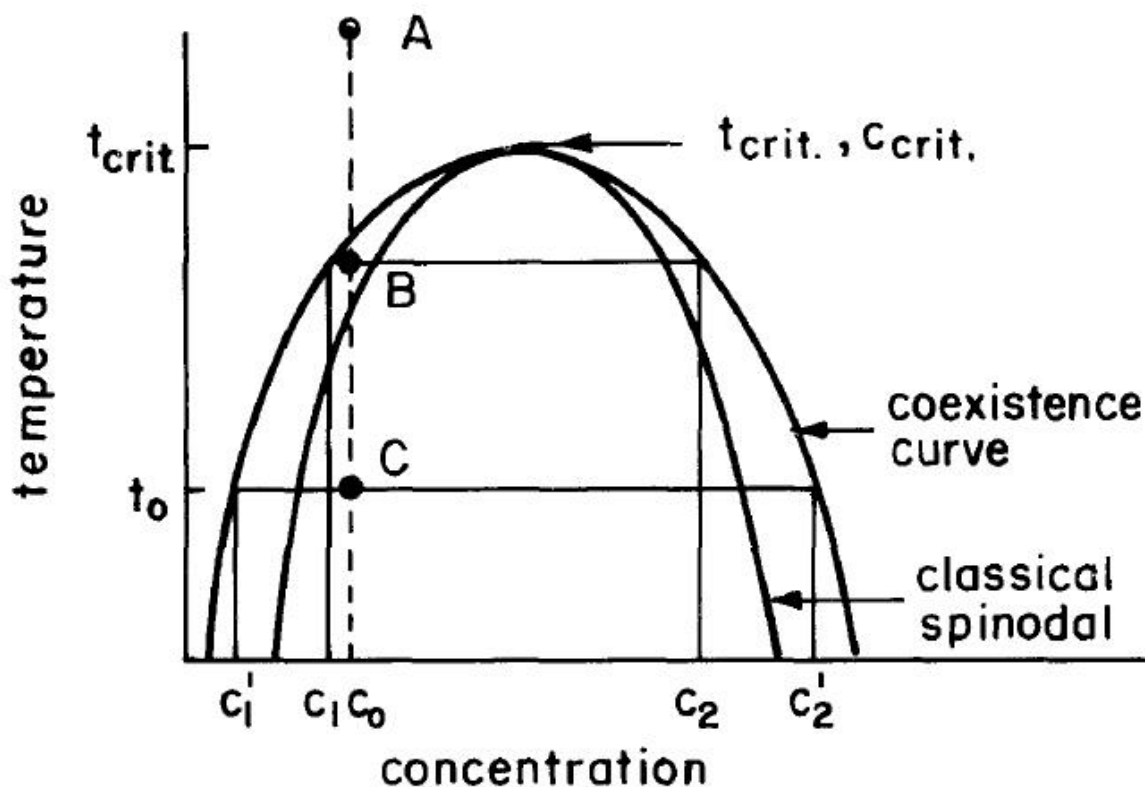


Figure 2.1:

The relaxation to equilibrium in non-isothermal systems is a process which can be characterized by coupling the Cahn-Hilliard equation with an equation for the temperature field. The resultant model is known as a conserved phase field model [12]. There are two curves in the phase diagram seen in Fig. 2.1 which help in understanding the phase separation. The outer (upper) curve is known as the binodal or the coexistence curve, and the inner or lower curve is known as the spinodal. These two curves intersect at the critical point, $(u_{crit}, \theta_{crit})$, where u_{crit} is the critical concentration and θ_{crit} is the critical temperature. If both the initial point (\tilde{u}, θ_0) and the final point (\tilde{u}, θ_1) lie above the binodal, the mixture is expected to persist in its initially uniform state, i.e. no phase separation is

expected to occur and $u(x, t) \equiv \tilde{u}$. This means that the region above the binodal corresponds to a stable or one phase region, [29]. Thus initiation of phase separation is determined by whether the initial state (\tilde{u}, θ_0) is above or below the binodal and spinodal, and whether the final state (\tilde{u}, θ_1) is under (below) the binodal, and above or below the spinodal. If (\tilde{u}, θ_1) lies below the spinodal curve and $u \approx u_{\text{crit}}$, then the phase separation is predicted to take place and to proceed by spinodal decomposition. During spinodal decomposition, the mixture is distinguished by a certain "fogginess" reflecting the simultaneous growth of many perturbations with many different wave lengths. If (\tilde{u}, θ_1) lies below the binodal but above the spinodal, phase separation can be expected to occur via nucleation and growth. In this case, phase separation occurs through the appearance of nuclei, or grains which persist and grow if they are large enough. In term of existence, the following result may be stated.

Theorem: Let $\Omega \subset \mathbb{R}^n, n \in \mathbb{N}$ where $\partial\Omega \in C^{1,1}$ or Ω is convex. Suppose that $u_0 \in H^1(\Omega)$ and $0 \leq u_0 \leq 1$, Then there exists a pair of functions (u, J) such that

- (a) $u \in L^2(0, T; H^2(\Omega)) \cap L^\infty(0, T; H^1(\Omega)) \cap C([0, T]; L^2(\Omega))$,
- (b) $u_t \in L^2(0, T; (H^1(\Omega)))$,
- (c) $u(0) = u_0$ and $\nabla u \cdot n = 0$ on $\partial\Omega \times (0, T)$,
- (d) $0 \leq u \leq 1$ a.e. in $\Omega_T := \Omega \times (0, T)$,
- (e) $J \in L^2(\Omega, \mathbb{R}^n)$,

and

$$u_t = -\nabla \cdot J,$$

in the sense that u for all $\zeta \in L^2(0, T; H^1(\Omega))$,

$$\int_0^T \langle \zeta(t), u_t \rangle_{H^1, (H^1)'} = \int_{\Omega_T} J \cdot \nabla \zeta,$$

and

$$J = -M(u)\nabla(-\epsilon^2 \Delta u + f'(u))$$

in the following weak sense :

$$\int_{\Omega_T} J \cdot \eta = - \int_{\partial\Omega_T} [\epsilon^2 \Delta u \nabla \cdot (M(u)\eta) + (Mf')(u)\nabla u \cdot \eta],$$

for all $\eta \in L^2(0, T; H^1(\Omega))$ which fulfill $\eta \cdot n = 0$ on $\partial\Omega \times (0, T)$. If $E(t)$ is defined as in (2 - 1 - 7), then for a.e. $t_1 < t_2$, where $t_1, t_2 \in [0, T]$, then

$$E(t_2) - E(t_1) \leq - \int_{t_1}^{t_2} \int_{\Omega} 1/M(u)|J|^2 dx.$$

The proof of the theorem is based on existence results for a regularized equation, in which the mobility is given by $M_\epsilon(u)$ and the free energy also depends on ϵ and is given by $f_\epsilon(u)$, and by establishing some estimates. For the Cahn-Hilliard equation the mean mass, $\bar{u} = \frac{1}{|\Omega|} \int u(x, t) dx$, is time invariant. The Cahn-Hilliard equation has no maximum principle.

Because the Cahn-Hilliard equation has a Lyapunov functional, namely the Van der Waals' free energy functional, and because this functional is decreasing along non-equilibrium orbits, the system is dissipative, and solutions can be expected to tend towards time independence as t becomes large, [23][12], i.e towards a steady state.

To understand thoroughly phase separation, let us consider for the moment the evolution of a system whose concentration is almost homogenous and spatially uniform which is cooled or quenched into a region in the thermodynamic phase diagram where the mean concentration is linearly unstable. Then the phase separation will commence producing a dominant length scale as predicted by the fastest growing or "most unstable" mode. This mode will be roughly apparent until the system locally saturates near the equilibrium phases or states. Afterwards, certain of the saturated regions will grow as others shrink, and the overall length scale of the system will gradually increase. This is the process called coarsening. Otto & Kohn [3] gave upper bounds on the dominant length scale during the coarsening, and A. Novick-Cohen & A Shishkov proved [22] a generalization valid for all temperatures. The process of phase separation in a two component system is accompanied by pattern formation and evolution. We should like to model the typical scenario of a quick quench by perturbing a uniform distributional of the two components,

$$u(x, 0) = u_0(x) \approx \bar{u}, \quad \bar{u} \in (0, 1).$$

This is undertaken in the next section.

2.2 Spinodal decomposition

Spinodal decomposition is a process by which a mixture of two or more materials can separate into distinct regions, with different composition. According to the Principle of Spinodal Decomposition [12], most solutions to the Cahn-Hilliard equation which start with initial data near a fixed constant concentrations in the spinodal region, exhibit fine-grained decomposition. Since this conjecture agrees with the outcome of physical experiment, the Cahn-Hilliard equation has been accepted as a meaningful model and fruitful means for describing the dynamics of phase transition. When a binary mixture is rapidly quenched to a lower temperature in a physical experiment, the sample which was initially spatially homogenous becomes inhomogeneous very quickly, decomposing into a fine grained alloy of particles where two distinct phases can be observed, with a characteristic length scale $\ell(t)$. This phenomenon is known as spinodal decomposition [12].

To understand how the history of the equation has developed, we note that while Van der Waals suggested in 1893 that the functional which appears in equation (2-1-6) was a good model for the free energy of binary mixtures, only sixty years later did Cahn and Hilliard rediscover this functional and derive the evolution equation induced by (2 – 1 – 2), through generalization of Fick's law of diffusion.

Moreover, they performed a linear analysis of (2 – 1 – 1) and argued that the results of this analysis suggested what we shall call the Principle of Spinodal Decomposition. The Cahn-Hilliard equation in its most familiar form may be written as in equation (2 – 1 – 6), where

$$f'(u) = -u + u^3,$$

namely as

$$u_t = \nabla^2(-u + u^3 - \varepsilon^2 \nabla^2 u). \quad (2 - 2 - 1)$$

The behavior of the evolution of this equation for small perturbations from spatial uniformity can be expressed by considering initial condition of the form

$$u_0(x) = \bar{u} + \tilde{u}_0(x), \quad (2 - 2 - 2)$$

and one can seek solutions of the form $u(x, t) = \bar{u}(x, t) + \tilde{u}(x, t)$. Substitution of these assumptions into (2 – 2 – 1) yields

$$\tilde{u}_t = M_0[-\tilde{u} + (\bar{u} + \tilde{u})^3 - \varepsilon^2 \tilde{u}_{xx}]_{xx}, \quad (x, t) \in \Omega_T, \quad (2 - 2 - 3)$$

where M_0 is a constant, and

$$\tilde{u}_x = M_0[-\tilde{u} + (\bar{u} + \tilde{u})^3 - \varepsilon^2 \tilde{u}_{xx}]_x, \quad (x, t) \in \partial\Omega_T, \quad (2 - 2 - 4)$$

$$\tilde{u}_0(x, 0) = \bar{u} + \tilde{u}_0(x), \quad x \in \Omega.$$

After linearization, we obtain

$$\tilde{u}_t = -M_0(u)[-(1 - 3\bar{u}^2)\tilde{u} - \varepsilon^2 \tilde{u}_{xx}]_{xx}, \quad (x, t) \in \Omega_T,$$

$$\tilde{u}_x = -M_0(u)[-(1 - 3\bar{u}^2)\tilde{u} - \varepsilon^2 \tilde{u}_{xx}]_x = 0, \quad (x, t) \in \partial\Omega_T, \quad (2 - 2 - 5)$$

$$\tilde{u}(x, 0) = \tilde{u}_0(x).$$

By neglecting terms multiplied by ε^2 , this approximation leads us to the "diffusion equation" with Neumann boundary condition

$$\tilde{u}_t = D\tilde{u}_{xx}, \quad (x, t) \in \Omega_T, \quad (2 - 2 - 6)$$

where $D = -M_0(1 - 3\bar{u}^2)$, and

$$\tilde{u}_x(x, t) = 0, \quad (x, t) \in \partial\Omega_T,$$

$$\tilde{u}(x, 0) = \tilde{u}_0(x), \quad x \in \Omega. \quad (2 - 2 - 7)$$

Using the familiar and standard separation of variation method, we get the general solution which corresponds to the solution of the classical diffusion equation, based on a negative diffusion coefficient. This equation is also known as the backwards diffusion equation, i.e. the equation obtained from

the classical diffusion equation via the transformation $t \rightarrow -t$. The solution using the method of separation of variables is based on looking for solutions of the form

$$u(x, t) = X(x)T(t), \quad (2-2-10)$$

and identifying solutions which are not trivial, i.e. do not equal to zero, which satisfy the given boundary conditions of the system. This technique for such problems generally yields Fourier series or generalized Fourier series.

Thus the diffusion equation which was originally derived by Adolf Fick in 1855 can be considered a special case of the Cahn-Hilliard equation. Substituting (2-2-10) into the diffusion equation yields

$$X(x)T'(t) = DX''(x)T(t) \quad (2-2-11)$$

which implies that

$$X''(x)/X(x) = T'(t)/DT(t) = -k \quad (2-2-12)$$

Since the RHS and the LHS of the above equation are functions of different independent variables, this implies that the two sides equal a constant k , and thus

$$X'' + kX = 0. \quad (2-2-13)$$

Equation (2-2-7) with the appropriate boundary condition, namely, $X'(0) = X'(L) = 0$, where L denotes an appropriate place, constitutes a Sturm-Liouville problem, whose solutions can be used in constructing solutions to (2-2-7).

Another way to proceed is by solving the diffusion equation using Green functions. For simplicity let us consider some one dimensional (1-D) solutions.

Case (i): The heat equation on the whole real line,

$$u_t = Du_{xx}, \quad -\infty < x < \infty, \quad 0 < t < \infty, \quad (2-2-14)$$

$$u(x, 0) = g(x), \quad -\infty < x < \infty, \quad 0 < t < \infty,$$

$$u(x, 0) = g(x), \quad -\infty < x < \infty,$$

whose solution is given by

$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} \int_0^\infty \exp(-(x-y)^2/4Dt)g(y) dy. \quad (2-2-15)$$

Case (ii): The heat equation of the half line

$$u_t = Du_{xx}, \quad 0 < x < \infty, \quad 0 < t < \infty,$$

$$\begin{aligned}
u(0, t) &= 0, \quad 0 \leq t < \infty, \\
u(x, 0) &= g(x), \quad 0 \leq x < \infty,
\end{aligned}$$

whose solution is given by

$$u(x, t) = \frac{1}{\sqrt{4\pi Dt}} \int_0^\infty (\exp(-(x-y)^2/4Dt) - \exp(-(x+y)^2/4Dt)) g(y) dy. \quad (2-2-16)$$

Case (iii). The heat equation on the half line with a source term,

$$u_t = Du_{xx} + f(x, t), \quad x \in R^+, t > 0,$$

$$\begin{aligned}
u(x, 0) &= 0, \quad x \in R^+, \\
u(0, t) &= 0, \quad t > 0,
\end{aligned}$$

whose solution is given by

$$u(x, t) = \int_0^t \int_0^\infty \frac{1}{\sqrt{4\pi D(t-s)}} \left(\exp\left(-\frac{(x-y)^2}{4D(t-s)}\right) - \exp\left(-\frac{(x+y)^2}{4D(t-s)}\right) \right) f(y, s) dy ds. \quad (2-2-17)$$

Returning to the method of separation of variables, one finds that the solution to (2-2-5) can be written as

$$\tilde{u}(x, t) = \frac{A_0}{2} + \sum_{n=1}^\infty A_n \exp^{-\frac{n^2\pi^2 D}{L^2} t} \cos(n\pi x/L), \quad (2-2-18)$$

where the coefficients $A_n, n = 0, 1, 2, \dots$, correspond to the Fourier coefficients of the initial condition,

$$A_n = \frac{2}{L} \int_0^L u_0(x) \cos\left(\frac{n\pi x}{L}\right) dx, \quad (2-2-19)$$

$$\tilde{u}(x, t) |_{t=0} = \tilde{u}_0(x) = \frac{A_0}{2} + \sum_{n=1}^\infty A_n \cos(n\pi x/L). \quad (2-2-20)$$

The solution approaches a constant at long time, $n = 0, 1, 2, \dots$

$$u(x, t) \rightarrow \frac{A_0}{2} \quad \text{as } t \rightarrow \infty.$$

Notice that its amplitude grows without bound, since

$$\|\tilde{u}(x, t)\|_{L^2[0, L]}^2 = \frac{A_0^2}{2} + \sum_{n=1}^\infty A_n^2 \exp\left(\frac{2n^2\pi^2 Dt}{L^2}\right). \quad (2-2-21)$$

In particular, for initial data based on a single mode, $\tilde{u}_0(x) = A_k \cos(k\pi x/L)$,

$$\|\tilde{u}(x, t)\|_{L^2[0, L]}^2 = A_k^2 \exp\left(\frac{2k^2\pi^2 Dt}{L^2}\right). \quad (2-2-15)$$

What we may deduce here is that the solution, under the assumption that $u(x, t) = \bar{u} + \tilde{u}(x, t)$, does not remain bounded within the interval $[0, 1]$ over time. This is an indication that the higher order terms proportional to ε^2 are necessary in order to get a more realistic physical model which can describe phase transition more accurately. Moreover, linear and numerical analysis have led to conjecture that a large class of solutions evolve relatively quickly to become nearly periodic with large amplitude and relatively small period. Such solutions appear to correspond to the experimentally observed phenomenon of spinodal decomposition, where the mixture dissociates into different phases after the alloy is rapidly quenched. The resultant characteristic length scale of the fine grained mixture grows and develops in size via a process called coarsening.

2.3 Coarsening

The Coarsening phenomenon.

A typical example of coarsening occurs in systems which exhibit phase transitions. During the late stages, the length scale of the system grows as certain of the regions dominated by one of the energy minimizing phases grow at the expense of the other. This process is known as coarsening, and often follows spinodal decomposition. In many technical applications [16], it is important to be able to predict the coarsening rate. To understand it from a phase separation point of view, let us consider the evolution of a system which is rapidly cooled or quenched into a region in thermodynamic phase diagram where the mean concentration is linearly unstable. Initially the fastest growing or most unstable mode will be apparent, then certain of the saturated regions will grow as others shrink, and the overall length scale of the system will slowly increase. This is the process known as coarsening, which we are now going to discuss. In particular we shall explore a new upper bound for $\ell(t)$, the characteristic length, recently obtained by A. Novick-Cohen and A. Shishkov [22], which generalizes the results of Kohn and Otto. We emphasize that when a system is cooled below the critical transition temperature, interconnected domains of the two equilibrium phases form and grow with time (coarsen) so as to decrease the total interfacial area. The domain patterns exhibit interesting scaling dynamics in which the patterns at later times are statistically similar to the earlier patterns apart from a global change of scale. It is thus natural to focus on how the characteristic length scale $\ell(t)$ changes with time, and it turns out that $\ell(t)$ typically grows as a power of time. This algebraic growth is going to be explored in this work.

Proving rigorous upper bounds for the coarsening rates has been seen to be a powerful tool in two standard models of surface-energy-driven interfacial dynamics. The sharp-interface version of the Cahn-Hilliard equation with constant mobility is the Mullins-Sekerka problem which is associated originally with solidification. The Mullins-Sekerka problem is a non-local problem in that the motion of the surfaces cannot be ascertained without taking in consideration the behavior within the entire domain containing the interfaces [39]. For related literature on Mullins-Sekerka problem, one can read

[3, 29]. In the Mullins-Sekerka problem, the domain Ω contains time dependent interfaces γ_t , and it can be formulated in the following manner:

$$\Delta\mu = 0, \quad (x, t) \in \Omega \setminus \gamma_t, \quad (2-3-1)$$

where γ_t denotes the interfaces, and along the interfaces γ_t ,

$$V = -[n \cdot \nabla(\mu)]_+^+, \quad (2-3-2)$$

where $V = V(x, t)$ denotes the normal velocity at the point $(x, t) \in \gamma_t$, and $n = n(x, t)$ denotes the unit exterior normal to γ_t , and μ denotes the classical potential,

$$\mu = -\kappa, \quad (2-3-3)$$

where κ denotes the mean curvature of γ_t . Along the external boundary of $\Omega \setminus \gamma_t$,

$$n \cdot \nabla\mu = 0, \quad x \in \partial\Omega.$$

Moreover γ_t perpendicularly intersects the boundary of $\partial\Omega$, namely $\gamma_t \perp \partial\Omega$. The chemical potential, $\mu = \mu(x, t)$, in the context of the Cahn-Hilliard equation formulation can be identified as

$$\mu = f'(u) - \varepsilon^2 \Delta u, \quad (2-3-4)$$

The Mullins-Sekerka problem and motion by surface diffusion, both preserve volume and decrease surface energy. The difference between them lies in that the mechanism of rearrangement in the Mullins-Sekerka corresponds to diffusion through the bulk, while surface diffusion corresponds to diffusion along the interfacial layer [3].

We are trying in this thesis to extract from [2, 3] precise estimates for free upper bound for coarsening for the degenerate Cahn-Hilliard equation in order to predict with high accuracy the algebraical power law behavior. Usually, coarsening phenomena are the result of phase separation which produced fine grains composed of two distinct phases. This process is known as spinodal decomposition, and the system separates into spatial regions rich in one component and poor in the other. After spinodal decomposition the mixture-alloy is fine grained.

The Cahn-Hilliard equation can also be obtained via Mean Field Theory based primarily on statistical mechanics, similar to the manner in which one gets the Ising model, when there is no mass conservation law. In magnetic systems an important quantum mechanical property is the spin directions. If the spins are parallel to the magnetic field, this is called a ferromagnetic response, while if they are anti-parallel the system is called paramagnetic. For phase transition based on a conserved order parameter, for example phase separation of a binary liquid, a growth "exponent" of $n = 1/3$ has been predicted by theory [5, 30], and a growth exponent $n = 1/2$ has been predicted for systems with

a non-conserved order parameter. Phase ordering kinetics is often described by universal growth laws of the form $\ell(t) \propto t^n$ where $\ell(t)$ is the characteristic length.

Another mathematical question which seems interesting is the existence of unique solutions to the Cahn-Hilliard equation, given smooth initial data. For the degenerate case uniqueness may not hold. The existence proof relies heavily on the existence of a Lyapunov functional, namely, the free energy functional, given in (2-3-5), which acts as a Lyapunov functional that can be expressed in the following form:

$$F[u] = \int d^n x \left[\frac{1}{4}(u^2 - 1)^2 + \frac{\epsilon}{2} |\nabla u|^2 \right] \quad (2-3-5)$$

which satisfies

$$dF/dt = - \int d^n x |\nabla \mu|^2 \leq 0. \quad (2-3-6)$$

Notice that the free energy functional contains two terms. The first term is the homogenous free energy which typically has the form of double well potential

$$f(u) = \frac{1}{4}(u^2 - b^2)^2 \quad (2-3-7)$$

with a constant $b \in (0, 1)$. To be more precise, in a mean field model [7], it assumes the form.

$$f(u) = \frac{\theta}{2} \left(u \ln(u) + (1-u) \ln(1-u) \right) + u(1-u) \quad (2-3-8)$$

which gives rise to a double-well potential when $\theta < 1$. Other forms of the free energy are possible, if $0 \ll \theta < 1$, (2-3-8) can be approximated by

$$f(u) = \frac{1}{4} u^2 (1-u)^2,$$

which has the advantage of being smoothly defined for all $u \in R$.

During the evolution from the initial condition, the domain Ω splits into three different types of subdomains. Two types of domains, Ω_0 and Ω_1 , are given by points where the solution is close to the minima of f where the binary mixture is rich in one component and poor in the other, as was mentioned before. A third type of domain is formed by thin transition layers, where the solution rapidly changes from being rich in one component to being poor in the other component.

As the interface width goes to zero, the resulting curve moves according to some geometric motion law [40]. which can be obtained by the method of formal asymptotic expansions via the scaling

$$t \rightarrow \zeta^2 t \quad \epsilon = \zeta^2, \quad \theta = \mathcal{O}(\epsilon^\alpha), \quad \alpha > 0, \quad (2-3-9)$$

For the degenerate Cahn-Hilliard equation in the limit $\zeta \rightarrow 0$, the interface moves by a geometric motion law called surface diffusion as mentioned in the previous chapter. Surface diffusion may be

expressed in terms of the normal velocity V and the mean curvature of the interface, κ , via the following relations

$$V = -\frac{\pi^2}{16}\Delta_s\kappa \quad (2-3-10)$$

$$n \cdot \nabla_s \kappa = 0, \quad x \in \gamma \cap \partial\Omega. \quad (2-3-11)$$

where Δ_s is the Laplace-Beltrami operator. This is in contrast to the constant mobility case, where we get the Mullins-Sekerka problem when $\zeta \rightarrow 0$ for rescaling time $t \rightarrow \zeta t$.

It should also be noted that the integral of the solution of equation (1-1-2) is preserved i.e.

$$\frac{d}{dt} \int_{\Omega} u dx = 0. \quad (2-3-12)$$

This property of the solution is important for image processing as one of the Cahn-Hilliard equation applications.

The second term in the free energy functional describes the interfacial energy of the system, and it is assumed that the parameter, ε^2 , is positive which implies that spatial gradients are penalized [7]. The effect of this term is that the total amount of transition zones is accounted for in the energy. This easily can be made precise in the limit when the thickness of the interface tends to zero [37]. Since $F[u]$ can be expected to be near to zero, this also indicates segregation into the domains, Ω_0 , Ω_1 as typical asymptotic outcome of the evolution of this equation. The segregation of such binary mixtures is characterized by transition layers between the segregated domains with a normal profile given by the function

$$u_e(x) = \tanh\left(\frac{x}{\varepsilon\sqrt{2}}\right) \quad (2-3-13),$$

where x denotes a locally defined normal coordinate to the interface. From this result it follows that interfaces have typical width $O(\varepsilon)$. Note that the function $u_e(x)$ is an equilibrium solution of the Cahn-Hilliard equation. The dynamics of coarsening is very attractive to study numerically via computer simulation or by analytical studies. It can be demonstrated at long times that $C \leq EL$. This result can be used to investigate upper bounds.

In general, when there is a phase transition below critical temperature, topological defects can be noticed at the interface between the two regions (fields). In a very large system, such as to the Universe in its early stages, topological defects occurred causing spontaneous symmetry breaking. Modern cosmological theory – the inflationary scenario – infers that magnetic monopoles, cosmic strings, domain walls and some other textures are direct result of such phase separation or transition. But in our case, there is no need to consider symmetry breaking since there is no natural "point space group". Hence in fluid mixtures, there is no need to take the topological symmetry in account.

In addition, R. V. Kohn and X. Yau [15] gave a model for coarsening rates for multi-component phase separation with both constant and degenerate mobility, and for an epitaxial growth model represented by a PDE equation. A heuristic argument suggests a coarsening rate of $t^{1/3}$, and R. V. Kohn & Xiaodong Yau showed that the system can coarsen no faster than $t^{1/3}$.

Chapter 3

The Cahn-Hilliard equation - basic properties

3.1 Cahn-Hilliard equation as a mathematical model

The very familiar Cahn-Hilliard equation

$$u_t = \Delta(-u + u^3 - \varepsilon^2 \Delta u), \quad (3-1-1)$$

and the less familiar Cahn-Hilliard equation

$$u_t = \nabla \cdot M(u) \nabla \cdot [\theta(\ln u - \ln(1-u)) - \alpha u - \varepsilon^2 \Delta u], \quad (3-1-2)$$

can both be written in the following form

$$u_t = \nabla \cdot M(u) \nabla \mu, \quad (3-1-3a)$$

$$\mu = f'(u) - \varepsilon^2 \Delta u. \quad (3-1-3b)$$

In both cases, constant and degenerate mobility, it makes sense to impose Neumann boundary condition, $n \cdot \nabla u = 0$, as well as the boundary conditions, $n \cdot \vec{j} = 0$, where

$$\vec{j} = M(u) \vec{\nabla} \mu(x, t), \quad (3-1-4)$$

which guarantees mass conservation. It is also possible to consider periodic boundary conditions, for the unknown function $u(t, x)$.

Let us again consider the perturbed Cahn-Hilliard equation as it appeared in (2-2-4), taking into consideration the linear part only, and neglecting the non-linear perturbative terms. Additionally we neglect also terms multiplied by ε^2 . This yields the following problem, [12]

$$\tilde{u}_t = -M_0(1 - 3\tilde{u}^2)\tilde{u}_{xx}, \quad (x, t) \in \Omega_T, \quad (3-1-5)$$

$$\tilde{u}_x = -M_0(1 - 3\bar{u}^2)\tilde{u}_{xx} = 0, \quad (x, t) \in \partial\Omega_T, \quad (3-1-6)$$

$$\tilde{u}(x, 0) = \tilde{u}_0(x), \quad x \in \Omega.$$

Under the assumption that $(3\bar{u}^2 - 1) < 0$, we obtain the classical diffusion equation with Neumann boundary conditions, which can be written as follows:

$$u_t = k\tilde{u}_{xx}, \quad (x, t) \in \Omega_T, \quad (3-1-7)$$

$$\tilde{u}_x = 0, \quad (x, t) \in \partial\Omega_T,$$

$$\tilde{u}(x, 0) = \tilde{u}_0(x), \quad x \in \Omega,$$

which does not undergo phase separation. And if $k = (1 - 3\bar{u}^2) > 0$, we obtain the backwards diffusion equation $\tilde{u}_t = -k\tilde{u}_{xx}$, whose solution we saw in chapter 2. Thus in both cases solving these problem makes partial physical sense. In the backwards diffusion equation, the higher order terms proportional to ε^2 are necessary in the physical model, and cannot be neglected. This provides a compelling reason to include such regularizing terms. We recall that such regularizing terms were already added much before the dynamics for phase separation came under consideration, when equilibrium consideration lead to the search for a free energy with phase separated steady states possessing certain regularity and uniqueness properties, notably in the pioneering work by Van der Waals (1873) and Gibbs (1893). For the Cahn-Hilliard equation, the regularizing terms are necessary in order to guarantee existence, uniqueness, stability, and bounded solutions in a framework which also guarantees finding numerical solutions.

3.2 Main results for the C-H equation

Linear Analysis: For $\Omega = [0, 1]$, the one dimensional Cahn-Hilliard equation may be written as

$$u_t = -(\varepsilon^2 u_{xx} - f'(u))_{xx}, \quad x \in (0, 1), \quad (3-2-1)$$

$$u_x = u_{xxx} = 0, \quad x \in [0, 1].$$

If the mean concentration \bar{u} lies in the spinodal region, then linearizing the equation about $u = \bar{u}$ gives

$$u_t = -\varepsilon^2 u_{xxxx} - \beta^2 u_{xx}, \quad x \in (0, 1), \quad (3-2-2)$$

where $\beta^2 := -f'(\bar{u}) > 0$.

The eigenfunctions of

$$u_{xx} + \lambda u = 0, \quad x \in (0, 1),$$

$$u_x(0) = u_x(1) = 0,$$

are

$$\cos n\pi x, \quad n = 0, 1, 2, \dots$$

The growth rate for the Fourier modes $\cos n\pi x$, $n = 0, 1, 2, \dots, n$ in the context of (3-2-2) is given by λ_n where

$$\lambda_n = (n\pi)^2[\beta^2 - \epsilon^2(n\pi)^2]. \quad (3-2-3)$$

For $0 < n < \beta/(\epsilon\pi)$, $\lambda_n > 0$, the corresponding Fourier modes grow as time progresses in the linearized equation, while the other modes remain steady or shrink. Thus, for $\epsilon < \beta\pi$, spatially homogeneous equilibria in the spinodal region are linearly unstable.

3.3 Physical properties dealing with coarsening

As was discussed in the previous chapter, typically coarsening follows spinodal decomposition during the phase separation process. There is a large class of systems which undergo phase separation for which one should like to determine their growth exponents. Such systems can contain various topological defects such as domain walls, cosmic strings, magnetic monopoles and some textures. In modern cosmological theory, the inflationary scenario infers that all these objects are direct consequences of phase separation. Cooled systems produce such objects via nucleation and coarsening, and through symmetry breaking of the vector or tensor order parameter. Scientists believe that such objects occurred in the early universe, and understand the main steps of the coarsening dynamics that produce that structures, A. Bray, [5]. Despite this similarity, these phase transitions are unlike the phase transitions described by Cahn-Hilliard dynamics, as they take place in an extreme ultra high energy setting.

We shall now define a number of functionals of our motion. Let $E(t)$ denote the free energy of the functional system which at late times approximates the interfacial area per unit volume, which has the dimension of $\frac{1}{\text{length}}$. Similarly let $\ell(t)$ denotes a suitable negative norm of the order parameter, which has dimensions of length. It is then possible under appropriate assumptions, to demonstrate $E > C$ or $LE > C$, where C is a positive constant. As the system evolves, the interfacial area decreases. This implies that the energy of the system also decreases, i.e $E' < 0$. The following differential inequalities may be shown to hold:

$$(L')^2 < C(-E'),$$

for Mullins -Sekerka problems, and

$$(L')^2 < C(E(-E')),$$

for surface diffusion dynamics, as a consequence of the basic energy-dissipative structure of the dynamics. Similar dynamics may be shown to hold for the Cahn-Hilliard equation. Details will be given in the next chapter.

3.4 The viscous C-H equation

Viscosity is the property by which fluids demonstrate resistance to flow. It is also well known that decreasing the temperature of the fluid or cooling it leads to an increase in the value of the viscosity coefficient. The viscous Cahn-Hilliard equation, A. Novick-Cohen & R. Pego, (1986), may be written as

$$(1 - \alpha)u_t = \Delta[f'(u) - \varepsilon^2 \Delta u + \alpha u_t] \quad (3 - 4 - 1)$$

where $f(u)$ is a double well potential, $\alpha \geq 0$, and Ω is a bounded domain,

$$\Omega \subset R^n, \quad n = 1, 2, 3, \dots$$

Setting $\alpha = 0$, the viscous Cahn-Hilliard equation reduces to

$$u_t = \Delta[f'(u) - \varepsilon^2 \Delta u] \quad (3 - 4 - 2)$$

i.e. the classical Cahn-Hilliard equation. Setting $\alpha = 1$, we obtain

$$u_t = \varepsilon^2 \Delta u - f(u) + \frac{1}{|\Omega|} \int_{\Omega} f(u) dx \quad (3 - 4 - 3)$$

which is a nonlocal second order parabolic equation known as the nonlocal reaction diffusion equation. The same equations can be obtained from the free energy functional by looking at the appropriate constrained (mass-conserving) gradient flow of the functional. The equation one obtains depends on the choice of definition of the gradient flow. Gradient flow in the sense of the $H^{-1}(\Omega)$ inner product yields the Cahn-Hilliard equation, while gradient flow in the $L^2(\Omega)$ inner product leads to the non-local reaction diffusion equation given above (See C.M. Elliott & A.M. Stuart 1993).

The viscous Cahn-Hilliard equation possesses a global attractor which is compact, connected and consists of equilibria and orbits connecting them. In one space dimension the equilibria are isolated [36]. In higher dimension this is not in general the case. For the Cahn-Hilliard equation one knows, that there exists an inertial manifold [41] and inertial sets. By definition, the inertial manifold and inertial sets are finite dimensional, exponentially attracting, and contain the global attractor. As far as dependence of the attractors on α and \bar{u} , the mean mass is concerned, denoting by $A_{\alpha}^{\bar{u}}$ the attractor of the viscous Cahn-Hilliard equation in one space dimension for a given value of \bar{u} and a given interval $\Omega = [0, 1]$, where the dependence of the global attractors resulting from the mass constraint has been indicated explicitly, the following result may be stated.

Theorem : The sets $A_{\alpha}^{\bar{u}}$ are Hausdorff continuous with respect to α and \bar{u} at $\alpha = 1$ for $\bar{u} \in [-1, 1]$. The proof may be found in M. Grinfeld, A. Novick-Cohen, [42].

For the non-local reaction-diffusion equation, we also have the following result (see [3]).

Lemma : If $u(x, t)$ is a solution of non-local reaction-diffusion equation, then its lap number is non-increasing with time.

3.5 The convective Cahn-Hilliard equation

The convective Cahn-Hilliard equation has been proposed to describe the evolution of crystal surfaces which are unstable due to the anisotropy of the surface tension along the surface of the crystal during its growth stage. This "convective Cahn-Hilliard model" [20] is based on various physical assumptions, such as that the local normal velocity is a linear function of the local under-cooling:

$$v_n = \mu^{-1}(\theta_e - \theta_i),$$

where θ_e denotes the equilibrium temperature, and θ_i denotes local surface temperature. During the growth process the crystal surface tension affects the growth rate via its effect on the equilibrium temperature θ_e , which depends on the surface tension γ , via the local Gibbs-Thomson relation,

$$\theta_e = \theta_m(1 - GK/H).$$

Here H denotes the latent heat, K is the mean curvature, which has been defined so that for a convex crystal surface, $K > 0$, and $G := \gamma + \partial^2\gamma/\partial\beta^2$ is the surface stiffness, where γ is the normal, and β represents the angle between the normal and the curve. Thus, in the convective Cahn-Hilliard model both kinetic and thermodynamics effects are taken in consideration, as well as the effect of surface tension on the formation of crystal face growth. If $G < 0$, disturbances of the crystal surface lead to the energy decrease. Although the increase of the surface area gives a positive contribution to the surface energy, at the same time part of the surface may fragment yielding new direction with lower energy.

There are various physical phenomena which can be described by the convective Cahn-Hilliard model, such as phase transition in the presence of an external field [21]. If the growth driving force σ goes to 0, where σ denotes the surface energy, $\sigma := E(u_+) - E(u_-)$, then spinodal decomposition occurs in phase-separating system [2, 3] and coarsening dynamics are exhibited [26]. On the other hand, the growth of the driving force causes a transition from coarsening dynamics to a chaotic spatiotemporal behavior. If the driving force goes to infinity, one expects the evolution to be governed by the Kuramoto-Sivashinsky equation [27] which is somewhat similar to the Cahn-Hilliard equation.

3.6 Turbulent coupling of C-H with the Navier-Stokes equation

Taking into account the presence of hydrodynamic velocity fields such as occur in fluids can make the behavior of phase separation and coarsening during the final stages even more complicated than the corresponding process which occurs in solid alloys [12]. In fluid dynamics, turbulence or turbulence flow is a flow regime characterized by chaotic changes. Hydrodynamics can accelerate domain growth [14, 15]. The complexity of the motion is due to the large number of degrees of freedom and to the possible chaotic behavior of some of them. It will be more difficult to comprehend than if the

system had only two or three degrees of freedom. Nevertheless, turbulence and coarsening have been extensively investigated in shear flows [17], where coarsening becomes highly anisotropic, and in which the single-phase domain growth accelerates in the shear direction, while in the transversal direction the growth is arrested [18] or strongly slowed down, and the phase separation may be suppressed [14]. Numerical experiments show that coarsening arrest is a generic and robust phenomenon. In phase separation produced by continuous stirring, [15], the main issue is the competition between the thermodynamic forces, which drive the phase separation, and the fluid motion which tends to lead to mixing and domain break-up. For very high flow intensities, phase separation can be completely suppressed, due to the mixing of the components and inhibition of interface formation. In active mixtures with very low viscosities, such phenomena may be self-induced by feedback [19], the fluid responds vigorously to local chemical potential variations and the components may again be mixed. In some cases stirring may decrease and lower the critical temperature [20] producing a deeper quench, and phase separation in a nontrivial statistically stationary state may continue to evolve.

Chapter 4

Energy estimates for coarsening

4.1 Obtaining estimates for global energy minimum.

We wish to identify upper bounds for coarsening for the degenerate Cahn-Hilliard equation based on the results on the paper of A. Novick-Cohen & A. Shishkov, [22]. Under appropriate assumptions, we have the following result: For all $\theta \in [0, 1]$,

$$\frac{1}{|\Omega|} \int_{\Omega} (u_{\pm}^2 - u^2) dx \leq 2E + 2\theta \ln 2 \quad (4-1-1)$$

where E is defined by

$$E(t) := \frac{1}{2|\Omega|} \int_{\Omega} \left[|\nabla u|^2 + \left[\frac{\partial W}{\partial u} \right]^2 \right] dx. \quad (4-1-2)$$

Let us now replace E by $E = E_{\text{new}} + E_{\text{min}}$ in (4-1-1), where E_{min} corresponds to the minimum attainable value of E for some given value of \bar{u} and θ . i.e. $E_{\text{min}} = E_{\text{min}}(\bar{u}, \theta)$. Then

$$\frac{1}{|\Omega|} \int_{\Omega} (u_{\pm}^2 - u^2) dx \leq 2(E_{\text{new}} + E_{\text{min}}) + 2\theta \ln 2, \quad (4-1-3)$$

which implies that

$$\frac{1}{|\Omega|} \int_{\Omega} u_{\pm}^2 dx - \frac{1}{|\Omega|} \int_{\Omega} u^2 - 2E_{\text{min}} \leq 2E_{\text{new}} + 2\theta \ln 2. \quad (4-1-4)$$

The inequality (4-1-4) can be seen as being more precise than (4-1-1), since $\min E_{\text{min}} = 0$, whereas $\min E = E_{\text{min}}$.

4.2 Upper bound for coarsening

Kohn and Otto [3] obtained rigorous results on upper bounds for coarsening for the Cahn-Hilliard equation with constant mobility [11], and for the degenerate mobility Cahn-Hilliard equation, [22]. Periodic boundary conditions were assumed and the mean mass, \bar{u} was taken to be $1/2$. They demonstrated upper bounds for the dominant length scale during coarsening. More precisely they proved

that there exist constants C_α such that if $L^{3+\alpha} \gg 1 \gg E_0$ and $T \gg L^{3+\alpha}$, where E denotes a scaled free energy and L is a $W^{1,\infty}$ preudal norm of u , then

$$\frac{1}{T} \int_0^T E^{\varphi r} L^{-(1-\varphi)r} dt \geq C_\alpha T^{-r/(3+\alpha)} \quad (4-1-5)$$

for all (r, φ) , such that $0 \leq \varphi \leq 1$, $r < 3 + \alpha$, $\varphi \cdot r > 1 + \alpha$, $(1 - \varphi)r < 2$. Their results are based on three lemmas [22, 29], which should hold at long times when the system has sufficiently coarsened, [3]. The first lemma gives a bound of the form $d \leq EL$ where d is $O(1)$, the second lemma gives a differential inequality involving E and L , and the third lemma uses the results of the first two lemmas to obtain upper bounds. In fact, upper bounds for coarsening have been shown to hold for all temperatures $\theta \in (0, \theta_c)$, [22], within the context of the Cahn-Hilliard equation with degenerate mobility,

$$(CH) \begin{cases} u_t = \nabla \cdot (1 - u^2) \nabla \left[\frac{\theta}{2} \ln \left[\frac{1+u}{1-u} \right] - u - \Delta u \right], & (x, t) \in \Omega_T, \\ n \cdot \nabla u = 0, & (x, t) \in \partial\Omega_T, \\ n \cdot (1 - u^2) \nabla \left[\frac{\theta}{2} \ln \left[\frac{1+u}{1-u} \right] - u - \Delta u \right] = 0, & (x, t) \in \partial\Omega_T, \\ u(x, 0) = u_0(x), & x \in \Omega. \end{cases}$$

Our goal in this section is to reconstruct the upper bounds for Cahn-Hilliard equation based on the three basic lemmas which were demonstrated in [22] and which generalize the three lemmas which appear in [3]. We now state these three lemmas below which shall be used in the sequel.

The calculation of the upper bounds could be reconstructed by using the three following lemmas:

Lemma 1. Assuming that $0 < \theta < 1$ and $u_- < \bar{u} < u_+$, then for any $t \geq 0$,

$$1 \leq A + \min(B_1, B_2), \quad (4-1-6)$$

where

$$A = \frac{2^{5/2}}{(u_\pm^2 - \bar{u}^2)} \left[\left(\frac{5/u_+}{[\theta(1/6 + h_{\min})]^{1/2}} E(t) + 3 \frac{|\partial\Omega|}{|\Omega|} \right) L(t) \right]^{1/2},$$

$$B_1 = \frac{1}{(u_\pm^2 - \bar{u}^2)} \left[\frac{2E(t)}{\theta(1/6 + h_{\min})} \right]^{1/2}, \quad B_2 = \frac{2}{(u_\pm^2 - \bar{u}^2)} [E(t) + \theta \ln 2].$$

For a full proof of this lemma see [22].

Lemma 2. If $u(x, t)$ is a solution of Cahn-Hilliard equation, $0 < \theta < 1$ and $|\bar{u}| < 1$, then the following estimates hold for $t \geq 0$,

$$|\dot{L}|^2 \leq -(1 - u_\pm^2) \dot{E} - \left[\frac{2}{\theta(1/6 + h_{\min})} \right]^{1/2} E^{1/2} \dot{E}, \quad (4-1-7a)$$

$$|\dot{L}|^2 \leq -[(1 - u_\pm^2) + 2\theta \ln 2] \dot{E} - 2E \dot{E}. \quad (4-1-7b)$$

Lemma 3. Suppose that

$$|\dot{L}|^2 \leq -AE^\alpha \dot{E}, \quad 0 \leq t \leq T, \quad \alpha = 0, 1/2, \text{ or } 1.$$

i) If, moreover, $LE \geq B$, for $0 \leq t \leq T$, then

$$\frac{1}{T} \left[\int_0^T E^{\varphi r} L^{-(1-\varphi)r} dt + L(0)^{(3+\alpha)-r} \right] \geq \vartheta_1 T^{-\frac{r}{3+\alpha}}. \quad (4-1-8)$$

ii) If, moreover, $E \geq C$, for $0 \leq t \leq T$, then

$$\frac{1}{T} \left[\int_0^T E^{\varphi r} L^{-(1-\varphi)r} dt + L(0)^{2-(1-\varphi)r} \right] \geq \vartheta_2 T^{-\frac{(1-\varphi)r}{2}}. \quad (4-1-9)$$

where

$$\vartheta_1 = \vartheta_1(A, B, \alpha, r, \varphi),$$

$$\vartheta_2 = \vartheta_2(A, B, \alpha, r, \varphi).$$

From these three lemmas it is possible to predict upper bounds for coarsening. We proceed by identifying $\min(B_1, B_2)$, and determining which inequality gives the tighter bounds in Lemmas 1 and 2. We neglect boundary contribution for simplicity. Suppose that $B_1 = \min(B_1, B_2)$. If $B_1 < 1/2$, then Lemma 1 implies a bound of the form $EL \geq B$, and if $B_1 > 1/2$, a bound of the form $E \geq C$, is predicted. If moreover,

$$(u_{\pm}^2 - \bar{u}^3)B_1 < (1 - u_{\pm}^2)^2, \quad (4-1-10)$$

then Lemma 2 provides an estimate of the form with $\alpha = 0$, and if (4-1-10) holds with the opposite sign, an estimate is obtained with $\alpha = 1/2$. Suppose that $B_2 = \min(B_2, B_2)$. If $B_2 < 1/2$, Lemma 1 implies a bound of the form $EL \geq B$, and if $B_2 > 1/2$, a bound of the form $E \geq C$ is obtained. If

$$2E < (1 - \bar{u}_{\pm}^2) + 2\theta \ln 2, \quad (4-1-11)$$

an estimate is obtained with $\alpha = 0$, and if (4-1-11) holds with the other sign, an estimate with $\alpha = 1$ is obtained.

The inequalities in Lemma 2 may be considered as generalizations of the inequalities obtained in [3], namely

$$(\dot{L}^2) \lesssim -\dot{E}, \quad \text{in the constant mobility case,}$$

and

$$(\dot{L}^2) \lesssim E(-\dot{E}), \quad \text{in the degenerate mobility case.}$$

4.3 Energy levels

We now define a set of energy levels,

$$\begin{aligned}
E_{11} &= \frac{1}{8}u_{\pm}^4\Psi(1-\beta^2)^2, \\
E_{12} &= \frac{1}{2}\Psi(1-u_{\pm}^2), \\
E_{21} &= \frac{u_{\pm}^2}{4}(1-\beta^2) - \theta \ln 2, \\
E_{22} &= \frac{1}{2}(1-u_{\pm}^2) + \theta \ln 2, \\
E_{\pm} &= \frac{\left[1 - (4 \ln 2)\theta\Psi \pm \sqrt{1 - (8 \ln 2)\theta\Psi}\right]}{4\Psi},
\end{aligned}$$

where

$$\Psi := \theta \left[\frac{1}{6} + h_{\min} \right],$$

and

$$\beta^2 := \bar{u}^2/u_{\pm}^2 < 1.$$

These energy levels determines which inequalities hold in Lemmas 1 and 2, and can be used to conclude various upper bounds.

We may now estimate these various energy levels at a number of different parameter limits.

Let us suppose that we are near the deep quench limit. Then we may set $u_+ = 1 - \delta$, with $0 < \delta \ll 1$. Proceeding in this manner, we find that

$$\begin{aligned}
\theta &= \frac{-2}{\ln \delta}(1 - \delta) + O\left[(\ln \delta)^{-2}\right], \\
\Psi &= \frac{(1 + \delta)^3}{(1 - \delta)} + O(\ln[\delta]^{-1}), \\
E_- &= 8\frac{(1 + \delta)}{(1 - \delta)}\left[\frac{\ln 2}{\ln \delta}\right]^2 + O([\ln \delta]^{-3}), \\
E_+ &= \frac{1}{2}(1 - 4\delta + O(\delta^2)), \\
E_{11} &= \left[\frac{1}{8} + O(\delta)\right]^{-3}(1 - \beta^2)^2, \\
E_{12} &= 2\delta^2 + O(\delta^3), \\
E_{21} &= \frac{(1 - \delta)^2}{4}(1 - \beta^2) + O[\ln \delta]^{-1}, \\
E_{22} &= \delta + O(\delta^2).
\end{aligned}$$

Under the assumption that $1 - \beta^2 = O(1)$, we obtain [22]

$$0 < E_- < E_{12} < E_{22} < E_{11} < E_{12} < E_+.$$

Suppose now that we are just below the critical temperature, in the proximity of the shallow quench limit. Then $0 < 1 - \theta \ll 1$ and $0 < u_+ \ll 1$, which implies that

$$E_{21} < 0 < E_{11} < E_{12} < E_- < E_{22} < E_+,$$

since

$$\begin{aligned} E_{\pm} &= \frac{3}{2} - \ln 2 \pm \frac{3}{2} \sqrt{1 - \frac{4}{3} \ln 2} + O(u_{\pm}^2), \\ E_{11} &= \left(\frac{1}{48} u_{\pm}^4 + O(u_{\pm}^6) \right) (1 - \beta^2)^2, \\ E_{12} &= \frac{1}{12} + O(u_{\pm}^2), \\ E_{21} &= -\ln 2 + O(u_{\pm}^2), \\ E_{22} &= \left(\frac{1}{2} + \ln 2 \right) + O(u_{\pm}^2). \end{aligned}$$

A numerical analysis of these energy levels has been undertaken by A. Novick-Cohen, M. Gruzd, J. Rashed, A. Shishkov, [32], which yields new results for the coarsening upper bounds for the Cahn-Hilliard equation, and show the influence of the temperature and concentration dependence. The graphs Figs. 4.1-4.5 show energy versus concentration $u_{\pm} = u_{\pm}(\theta)$ at various different magnifications. In these graphs, u_+ is denoted by "u" and energy bounds E_{\pm} , E_{11} , E_{12} , E_{21} , E_{22} are portrayed. Upper bounds based on $EL \geq B$ are indicated as $\ell(t) \propto t^{\alpha}$, and upper bounds based on $E \geq C$ are indicated as $\ell(t) \propto t^{\alpha+}$. The graphs also show how the behavior of the upper bounds can be sensitive to small changes in u_{\pm} near the deep quench limit.

4.4 Some numerical results.

An approach to solve the Cahn-Hilliard equation numerically is to build an appropriate scheme which is based on finite element methods. Another approach is via finite difference method. Another method which can be used is the method of lines which yields an "ODE" system, [7]. Studies for the Cahn-Hilliard equation have done by H.Garcke et al., [37] who included the effects of elasticity in their computations and made use of finite element methods.

Numerical studies of Cahn-Hilliard equation with applications to image processing have been done by Vladimir Chalupecky [7]. In his, one can see the evolution of an initial shape with r "leaves," the boundary of which has been damaged by small bumps. The small bumps at the boundary are smoothed out quickly while the overall four-leaf shape almost does not change. Even after a long time,

the final shape does not differ much from the original one. In the letter "R," a similar effect takes place, see Fig. 4.6. The only difference is the amount of noise apparent in the boundary. Even though the boundary is now quite damaged, after a short time we get results which may be more suitable for further processing.

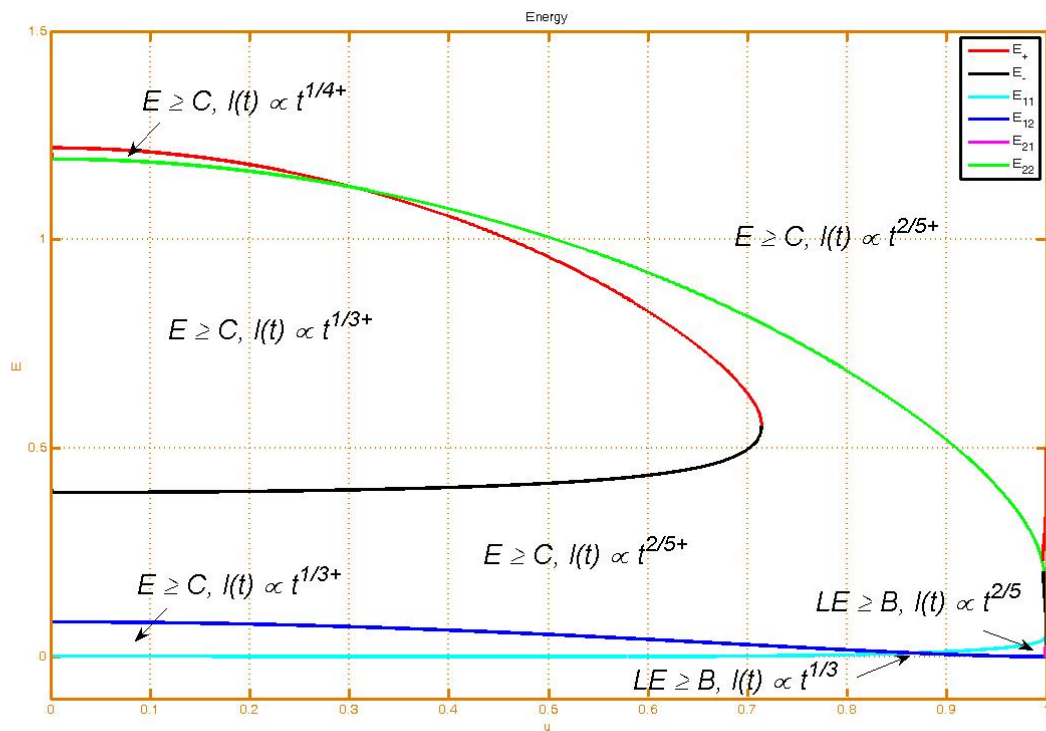


Figure 4.1:

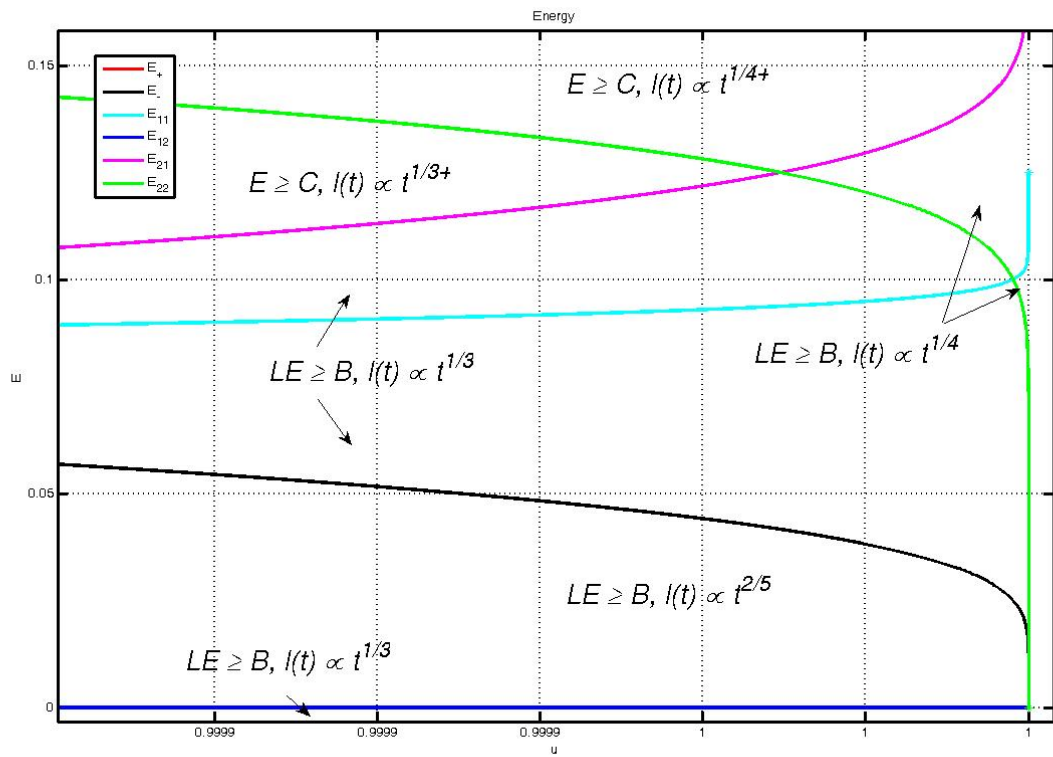


Figure 4.2:

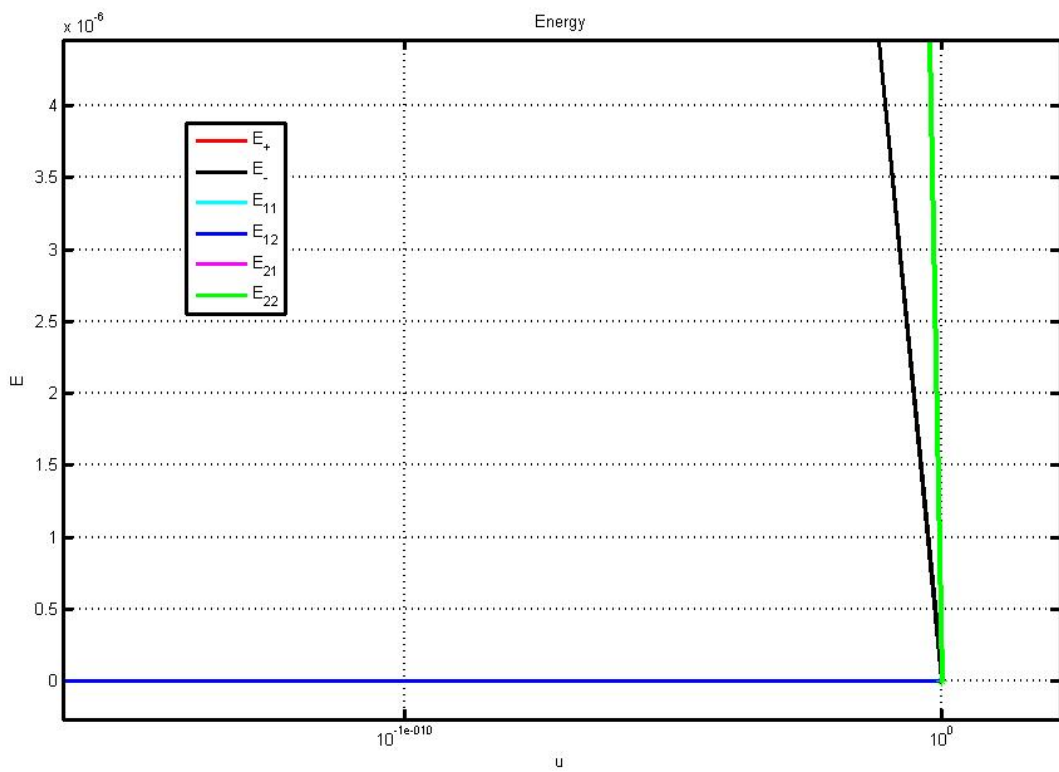


Figure 4.3:

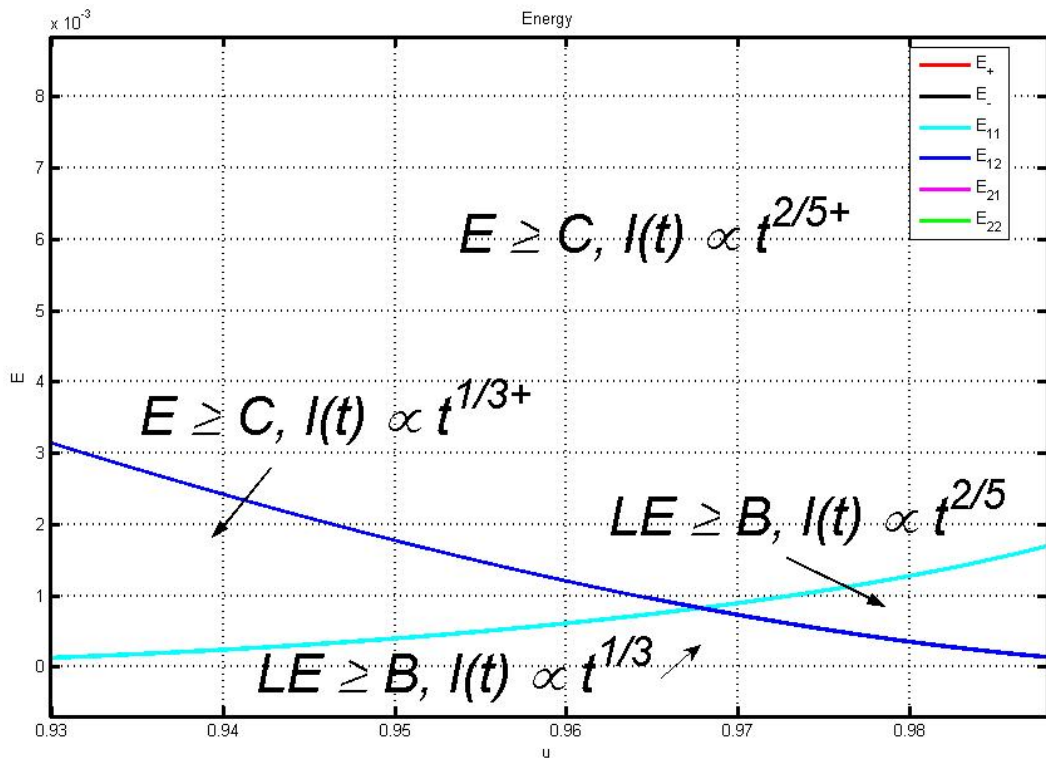


Figure 4.4:

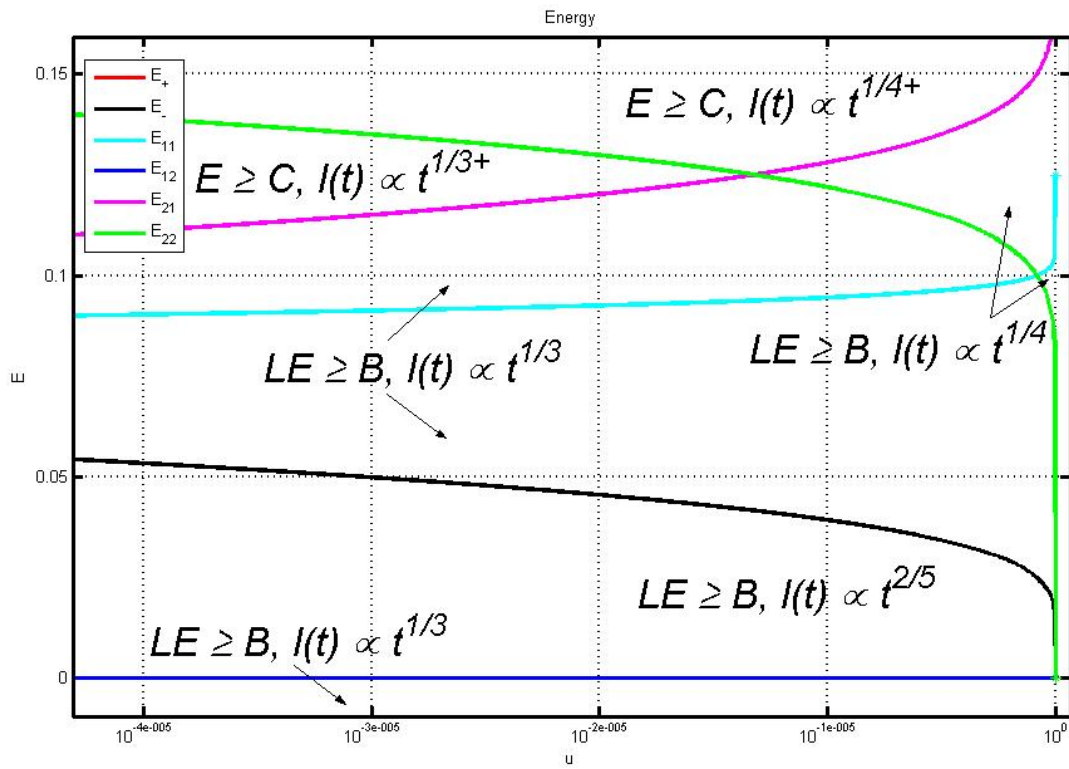
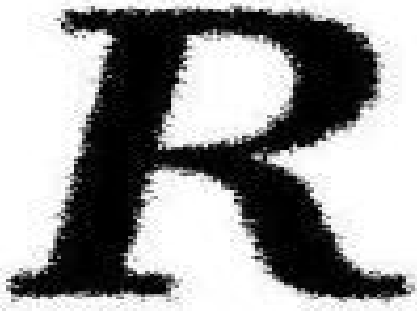


Figure 4.5:



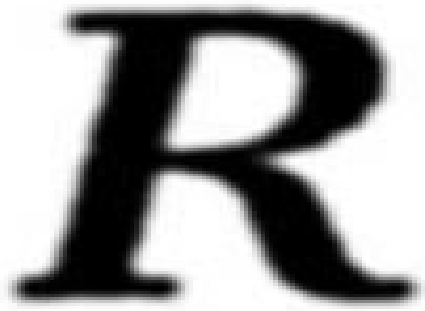
(a) $t = 0$



(b) $t = 2.5 \cdot 10^{-2}$



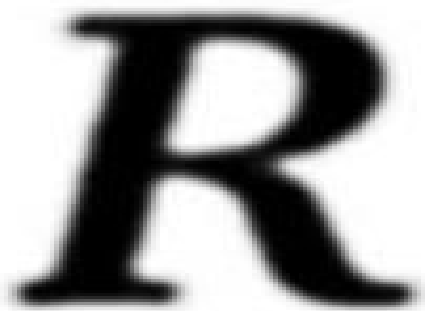
(c) $t = 5 \cdot 10^{-2}$



(d) $t = 10^{-1}$



(e) $t = 2.5 \cdot 10^{-1}$



(f) $t = 5 \cdot 10^{-1}$

Figure 4.6: Shape recovery

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