Allen-Cahn & Phase Transition Systems

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MSc Thesis

Athens, September 2025

This thesis is dedicated to my two sisters, for their constant support.

Acknowledgments

Abstract

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CHAPTER 1

The Allen-Cahn equation and underlying physics

The purpose of this chapter is to introduce the basic intuition and physics behind the Allen-Cahn equation, and also to briefly explore the related Cahn-Hilliard equation. Everything mentioned here is, in some way, classical and has more of a didactic or physical value than mathematical, so we will be brief. However, it sets the basis and the background for the next chapters to come.

First, we will describe the phenomenon of phase seperation in (two-component) alloys, which is modeled by a Reaction-Diffusion equation, called the parabolic Allen-Cahn equation. The important feature, and sort-of the selling point, of this Allen-Cahn equation is the modeling of co-existence of phases. The mentioned equation will appear by the interaction of a diffusion quantity with a potential. The time-invariant parabolic Allen-Cahn equation, or simply the Allen-Cahn equation, is basically an equation that yields time-invariant solutions of the parabolic Allen-Cahn equation. The latter are important, as they can be thought as a "balance point" after long (infinite) time.

Next, we will go back to 1975, to Allen's and Cahn's paper [4], in which the physics of the phenomenon of phase seperation is explored thorougly. This paper has historical value, as it is the first appearance of the paracolic Allen-Cahn equation in alloying.

Then, we will change our perspective and we will explore another physical phenomenon, which is modeled by the same equation, the Allen-Cahn equation, that is the phase transition in materials. Here the word "phase" is used by its usual meaning, which is something in the set {solid, liquid, gas, plasma}. Here the co-existence feature of the Allen-Cahn equation is of course important, as in some materials (such as in plain water) it has been experimentally proven that there exists "triple points", that is, points in phase space (temperature and pressure) in which it is possible to find solid, liquid and gas states simultaneously.

In the end, we will see the Allen-Cahn equation from an energy point of view. It is intuitive that the energy of such phenomena, and in partucular in the phase seperation in alloys, is dependent of the connecting surface (interface) between the components. So, the so-called stress-energy tensor will come into play, and we will show that the Allen-Cahn equation is in fact equivalent to the divergence-free condition of the stress-energy tensor.

1.1 Describing the formation and geometry of alloys

1.1.1 The mathematical formulation of the equation

The first phenomenon we will describe is the phase seperation in alloys. As the phenomenon we are dealing with is of Reaction-Diffusion type, we are expecting to find a diffusion term $\partial_t u = \Delta u$ as well as a potential W. However, it is important before we proceed to understand the role of the solution u, because the meaning we give to it influences the physical intuition and therefore the phenomenon.

In the case of two-component alloys, we suppose we have a mixture A of components A_1, A_2. We want to describe the quantity of A_1 and A_2 in a point of space, so u can be thought as a signed concentration, where -1 corresponds to pure phase A_1 and 1 to pure phase A_2. Intermediate values correspond to the existence of both A_1 and A_2.

Figure 1.1

In this case, $u : \mathbb{R}^n \to \mathbb{R}$ is a function from space to the reals. In the multi-component case, one dimension $\mathbb{R}$ does not suffice to explain the physics. This is some elementary geometry fact:

Figure 1.2

When three pure phases are put in a line, it is impossible to find a point that models the co-existence of all three phases. In this case, an extra dimension is needed, so u takes vector values. In this case, $u : \mathbb{R}^n \to \mathbb{R}^m$, $m \geqslant 2$.

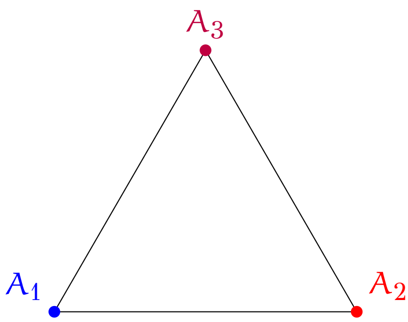

Figure 1.3

In more sophisticated examples, the ambient space is a Riemannian manifold. In general, u is a function $u : \mathscr{M} \to \mathbb{R}^m$, where $\mathscr{M}$ is an $n-$dimensional Riemannian manifold.

We now start with the diffusion, which is the expected movement if only one component is present. Let $\Omega \subseteq \mathscr{M}$ be an bounded open set of a Riemannian manifold with smooth boundary $\partial\Omega \in C^\infty$. The total concentration inside Ω is:

$$\int_\Omega u \, d\sigma$$

and the change of this concentration is $\partial_t \int_\Omega u \, d\sigma$. Because of diffusion, the concentration moves through the boundary $\partial\Omega$ and towards lower concentration. This means there exists a vector field F, such that the the flow of concentration through $\partial\Omega$ is dependent on:

$$\int_{\partial\Omega} \langle F, \widehat{n} \rangle \, dS, \text{ where } \widehat{n} \text{ is the unit normal vector field}$$

It is a usual convention to use $F = -\alpha \nabla u$, for some positive constant $\alpha > 0$. The minus sign is used so the flow is from higher to lower concentration.

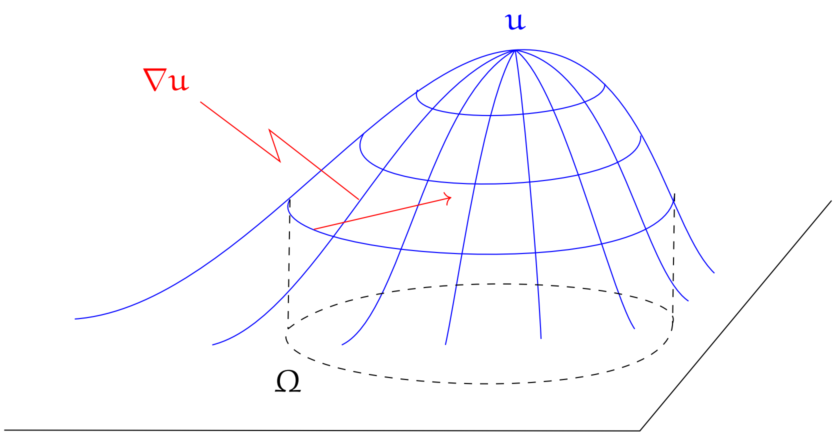

Figure 1.4

Because the total concentration is expected to decrease, we set:

$$\partial_t \int_\Omega u \, d\sigma = -\int_{\partial\Omega} -\alpha \langle \nabla u, \widehat{n} \rangle \, dS = \int_{\partial\Omega} \alpha \langle \nabla u, \widehat{n} \rangle \, dS$$

Now we would like to interchange the derivative with the integral. This is known to can be done, given adequate smoothness, but, in fact, almost no smoothness is needed to interchange the integral with the derivative. We note this in D.1. Doing the interchange, we arrive at:

$$\int_{\partial\Omega} \partial_t u \, d\sigma = \int_{\partial\Omega} \alpha \langle \nabla u, \widehat{n} \rangle \, dS = \int_{\partial\Omega} \alpha \nabla \bullet \nabla u \, d\sigma$$

(in the last equality we use the divergence theorem). This means:

$$\int_{\partial\Omega} \partial_t u - \alpha \Delta u \, d\sigma = 0 \text{ for all } \Omega \Rightarrow \partial_t u = \alpha \Delta u$$

As far as the potential goes, for the two-component case, one wants to use a potential that forces u to either -1 or to 1, that is to pure phases. So potential W must aquire two minima, at ± 1, and then the force on u is $-\nabla W = -W_u$.

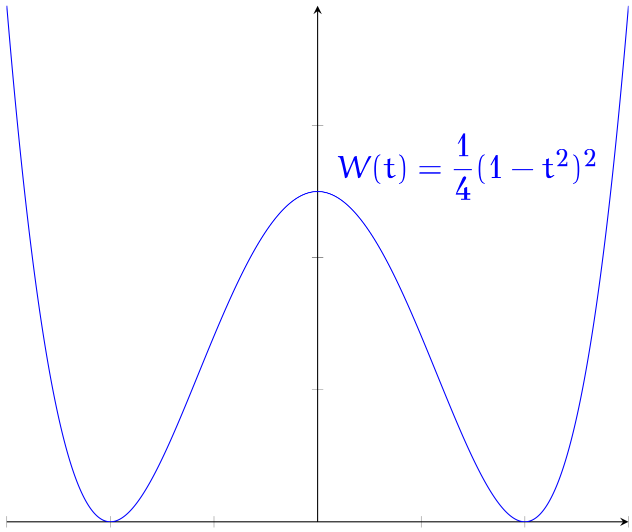

Figure 1.5

One usual choice for the potential W is $W(t) = \frac{1}{4}(1-t^2)^2$, the so-called Ginzberg-Landau potential. In the case of multicomponent alloys, W will be different, having multiple seperated minima. Connectedness of the set of minima of W is also important and can appear. It is usual for W to minimise to the zero value, but it is possible to have an unbalanced structure too.

In general, the parabolic Allen-Cahn equation is:

$$\partial_t u = \varepsilon^2 \Delta u - W_u(u)$$

which contains a diffusion term and a reaction term. If one deals with time-invariance, that is $\partial_t u = 0$, the parabolic Allen-Cahn equation is just the Allen-Cahn equation, $\varepsilon^2 \Delta u - W_u(u) = 0$. Time-invariance is modeling the phenomenon after infinite time, when the two terms have balanced one another.

1.1.2 Allen's and Cahn's original paper, and the physical perspective

More insight to the component seperation can be gained by studying the original paper from Allen and Cahn [4].

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CHAPTER B

Appendix: Geometry

In this appendix we briefly explain the theory of differentiable Riemannian manifolds. At first, we would dismiss this chapter, but after discussion with applied mathematicians on Festum-π conference, in Chania 2024, we realised that is important to make an elementary introduction, perticularly for the “applied mathematician”.

B.1 Manifolds with differential structure

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CHAPTER D

Appendix: Miscellaneous

Theorem D.1 (Integral and derivative interchange [10], [11]). *Let $\Omega \subseteq \mathbb{R}^n$ be an open set and $(X, \mathcal{M}, \mu)$ a measure space.*

i. Suppose we have a function $f(p,x)$ which is Lebesgue integrable in the first variable and for almost all $x \in X$ the derivatives $\partial_{p_i} f(p,x)$ exist for all $p \in \Omega$. If there exists an integrable function $\theta : X \to \mathbb{R}^n$ such that:

$$|\partial_{p_i}(p,x)| \leqslant |\theta(x)|, \text{ for all } p \in \Omega, \text{ almost every } x \in X$$

then for all $p \in \Omega$:

$$\partial_{p_i} \int_X f(p,x)\ d\mu = \int_X \partial_{p_i} f(p,x)\ d\mu$$

ii. We consider the family of classical distributions $\{f(p,x)\}_{x \in X}$ and we define:

$$\left\langle \int_X f(\cdot,x)\ d\mu, \varphi \right\rangle := \int_X \langle f(\cdot,x), \varphi \rangle\ d\mu, \ \ \varphi \in C_c^\infty(\Omega; \mathbb{R})$$

If the above is well-defined and gives a distribution, then:

$$\partial_{p_i} \int_X f(p,x)\ d\mu = \int_X \partial_{p_i} f(p,x)\ d\mu$$

where ∂_{p_i} is the generalised distributional derivative.

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